```
=> file reg
FILE 'REGISTRY' ENTERED AT 13:20:50 ON 11 FEB 2003
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=> d his

     FILE 'LREGISTRY' ENTERED AT 11:00:19 ON 11 FEB 2003
L1                STR
L2                STR L1

     FILE 'REGISTRY' ENTERED AT 11:20:14 ON 11 FEB 2003
L3              4 SEA SSS SAM L1 OR L2
L4                SCR 405 AND 1199 AND 1838 AND 1992
L5                SCR 1841
L6              6 SEA SSS SAM (L1 OR L2) AND L4
L7             11 SEA SSS SAM (L1 OR L2) AND L4 NOT L5
L8                SCR 1918 OR 2043 OR 2127 OR 2040 OR 2041 OR 2049
L9             10 SEA SSS SAM (L1 OR L2) AND L4 NOT (L5 OR L8)
L10               SCR 1066 OR 1130 OR 1195
L11            50 SEA SSS SAM (L1 OR L2) AND L4 AND L10
L12               STR L1
L13               STR L2
L14            50 SEA SSS SAM (L12 OR L13) AND L4 AND L10
L15         15873 SEA SSS FUL (L12 OR L13) AND L4 AND L10
                  SAV TEM L15 ASI953/A

     FILE 'HCA' ENTERED AT 13:01:17 ON 11 FEB 2003
L16          7108 SEA L15
L17          2040 SEA SOLIDPHAS?(2A)(SUPPORT? OR SYN# OR SYNTH# OR
                  SYNTHET?) OR SOLID?(3A)(PHASE# OR PHASING# OR SUPPORT?)(3
                  A)(SYN# OR SYNTH# OR SYNTHET?) OR SOLID?(3A)(PHASE# OR
                  PHASING#)(3A)SUPPORT?
L18          6723 SEA MERRIFIELD# OR WANG#
L19             2 SEA L16 AND L17
L20            14 SEA L16 AND L18
L21        121541 SEA SOLIDPHAS? OR SOLID?(3A)(PHASE# OR PHASING# OR
                  SUPPORT?)
L22           118 SEA L16 AND L21
L23               QUE SYN# OR SYNTH# OR SYNTHES!S? OR SYNTHETIC?
L24            73 SEA L22 AND L23
L25         13233 SEA (SOLIDPHAS? OR SOLID?(3A)(PHASE# OR PHASING# OR
                  SUPPORT?))(3A)(SYN# OR SYNTH# OR SYNTHES!S? OR SYNTHETIC?
                   OR SYNTHESIZ?)
L26            61 SEA L16 AND L25
L27            16 SEA L19 OR L20
L28            48 SEA L26 NOT L27


     FILE 'REGISTRY' ENTERED AT 13:20:50 ON 11 FEB 2003
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L10               SCR 1066 OR 1130 OR 1195
L12               STR
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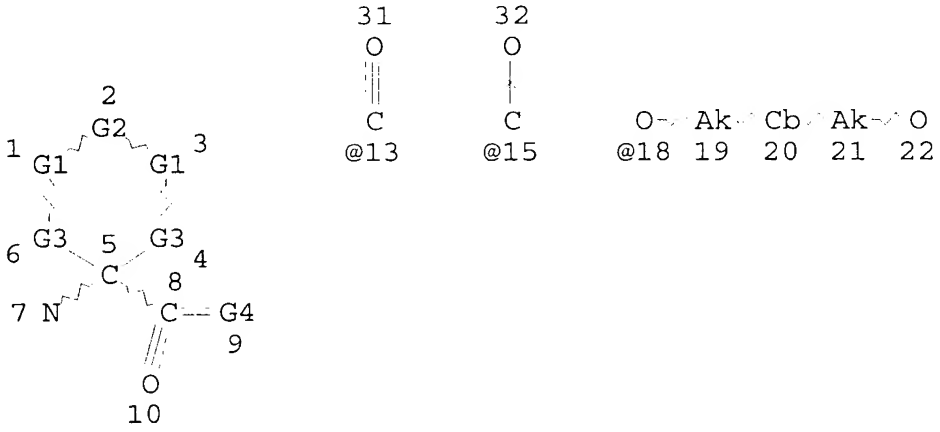


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GGCAT   IS UNS  AT  20
DEFAULT ECLEVEL IS LIMITED

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STEREO ATTRIBUTES: NONE
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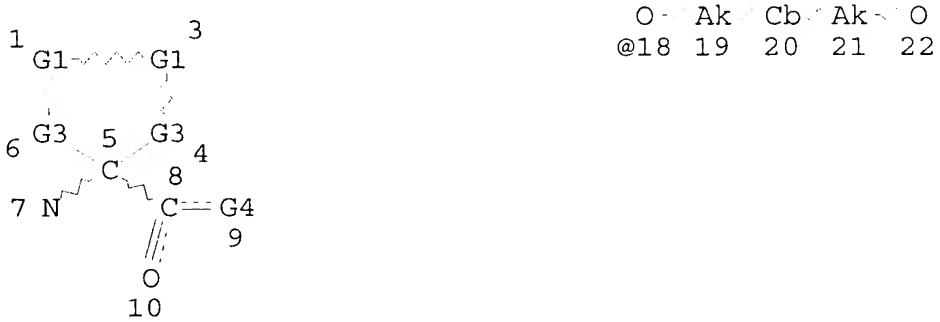


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REP G3=(0-2) C
VAR G4=O/NH/18
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GGCAT IS UNS AT 20
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE
L15 15873 SEA FILE=REGISTRY SSS FUL (L12 OR L13) AND L4 AND L10

100.0% PROCESSED 54699 ITERATIONS 15873 ANSWERS
SEARCH TIME: 00.00.04

=> file hca
FILE 'HCA' ENTERED AT 13:22:03 ON 11 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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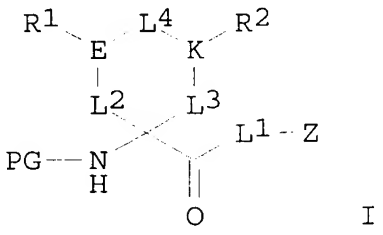
=> d l27 1-16 cbib abs hitstr hitind

L27 ANSWER 1 OF 16 HCA COPYRIGHT 2003 ACS
137:33218 Preparation of resin-bound cyclic quaternary amino acids. Dhanos, Dalijit (Pharmacore, Inc., USA). PCT Int. Appl. WO 2002046128 A2 20020613, 93 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US46585 20011206. PRIORITY: US 2000-PV251728 20001206.
GI



I

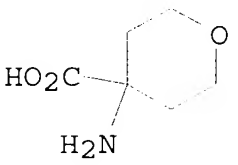
AB Resin-bound quaternary cyclic amino acids I (Z = polymer support; L1

= O, NH, 1,x-OCH2C6H4CH2O; L2, L3 = alkanediyl, alkenediyl, alkynediyl, single bond; L4 = alkanediyl, O, S, CO, SO, SO2, C(OCH2CH2O), C(OCH2CH2CH2O), single or double bond; E, K = N, CH, C; PG = H, amino protecting group; R1, R2 = alkyl, alkenyl, alkynyl, cycloalkyl, heterocyclyl, aryl, heteroaryl, H, halo, HO, substituted alkoxy, (un)substituted amino; R1R2 = cycloalkyl, heterocyclyl) are prepd. as solid-phase reagents for the prepn. of combinatorial libraries or in the prepn. of peptides and other compds. for drug discovery. (no data). Amino acids attached to both **Merrifield** and **Wang** resins are prepd.

IT **217299-03-1**
(prepn. of resin-bound cyclic quaternary amino acids)

RN 217299-03-1 HCA

CN 2H-Pyran-4-carboxylic acid, 4-aminotetrahydro-, hydrochloride (9CI) (CA INDEX NAME)

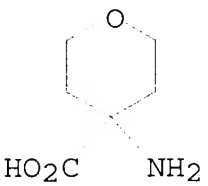


● HCl

IT **39124-20-4P 252720-31-3P 369403-17-8P**
369403-21-4P 436867-74-2P 436867-75-3P
(prepn. of resin-bound cyclic quaternary amino acids)

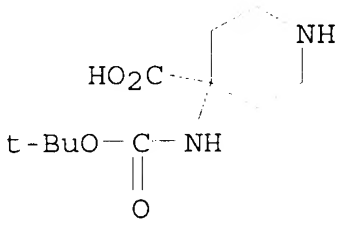
RN 39124-20-4 HCA

CN 2H-Pyran-4-carboxylic acid, 4-aminotetrahydro- (9CI) (CA INDEX NAME)

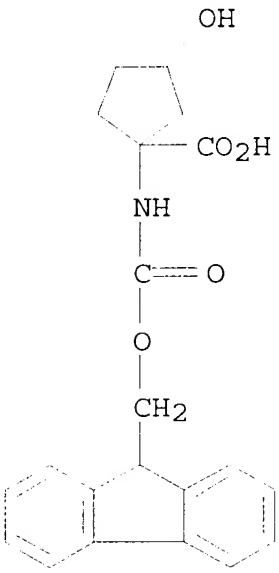


RN 252720-31-3 HCA

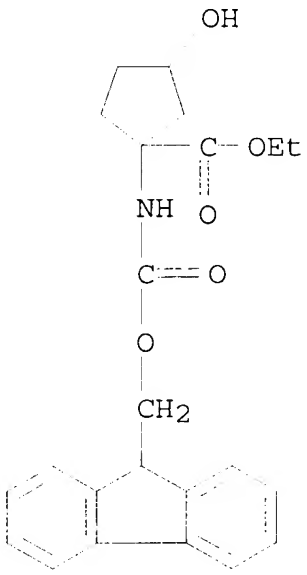
CN 4-Piperidinecarboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



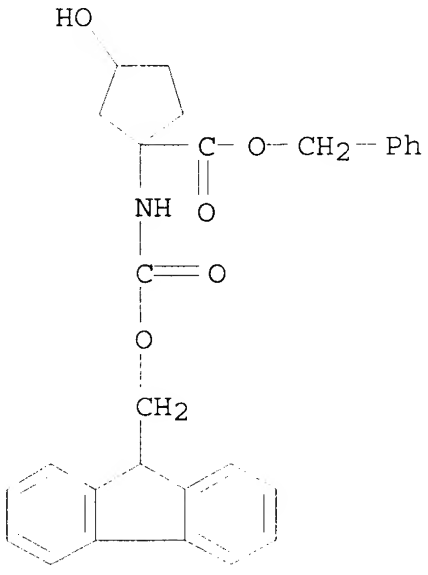
RN 369403-17-8 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-hydroxy- (9CI) (CA INDEX NAME)



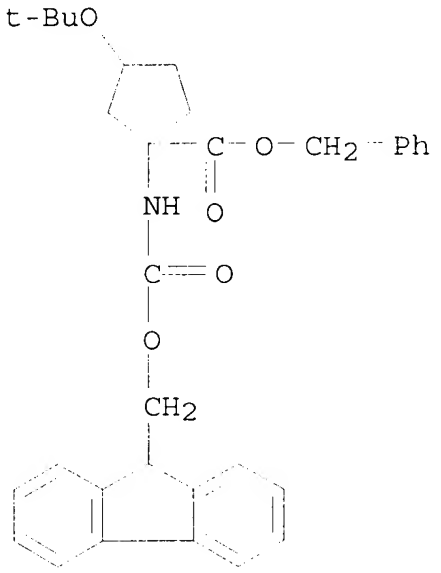
RN 369403-21-4 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



RN 436867-74-2 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-hydroxy-, phenylmethyl ester (9CI) (CA INDEX NAME)



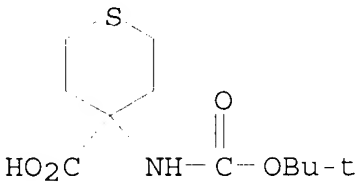
RN 436867-75-3 HCA
CN Cyclopentanecarboxylic acid, 3-(1,1-dimethylethoxy)-1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, phenylmethyl ester (9CI) (CA INDEX NAME)



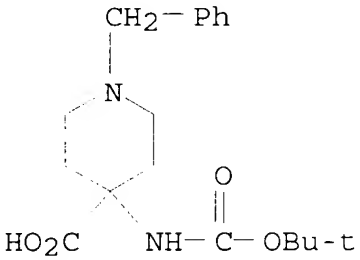
IT **108329-81-3DP**, **Wang** and **Merrifield** resin-bound **150435-81-7DP**, **Wang** and **Merrifield** resin-bound **162648-54-6DP**, **Wang** and **Merrifield** resin-bound **172843-97-9DP**, **Wang** and **Merrifield** resin-bound **172843-97-9P 183673-66-7DP**, **Wang** and **Merrifield** resin-bound **191110-68-6DP**, **Wang** and **Merrifield** resin-bound **252720-31-3DP**, **Wang** and **Merrifield** resin-bound **285996-72-7DP**, **Wang** and **Merrifield** resin-bound **285996-72-7P 368866-07-3DP**, **Wang** and **Merrifield** resin-bound **368866-07-3P 368866-19-7DP**, **Wang** and **Merrifield** resin-bound **368866-20-0DP**, **Wang** and **Merrifield** resin-bound **368866-21-1DP**, **Wang** and **Merrifield** resin-bound **368866-30-2DP**, **Wang** and **Merrifield** resin-bound **368866-35-7DP**, **Wang** and **Merrifield** resin-bound **369402-94-8DP**, **Wang** and **Merrifield** resin-bound **369402-96-0DP**, **Wang** and **Merrifield** resin-bound **369403-08-7DP**, **Wang** and **Merrifield** resin-bound **369403-10-1DP**, **Wang** and **Merrifield** resin-bound **369403-15-6DP**, **Wang** and **Merrifield** resin-bound **369403-15-6P 369403-17-8DP**, **Wang** and **Merrifield** resin-bound **369403-19-0DP**, **Wang** and **Merrifield** resin-bound **369403-24-7DP**, **Wang** and **Merrifield** resin-bound **436867-66-2DP**, **Wang** and **Merrifield** resin-bound **436867-67-3DP**, **Wang** and **Merrifield**

resin-bound **436867-68-4DP**, **Wang** and **Merrifield** resin-bound **436867-69-5DP**, **Wang** and **Merrifield** resin-bound **436867-70-8DP**, **Wang** and **Merrifield** resin-bound **436867-71-9DP**, **Wang** and **Merrifield** resin-bound **436867-72-0DP**, **Wang** and **Merrifield** resin-bound **436867-73-1DP**, **Wang** and **Merrifield** resin-bound
(prepn. of resin-bound cyclic quaternary amino acids)

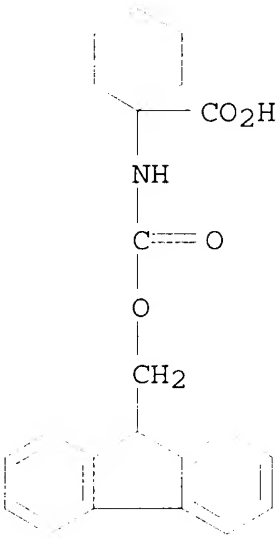
RN 108329-81-3 HCA
CN 2H-Thiopyran-4-carboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]tetrahydro- (9CI) (CA INDEX NAME)



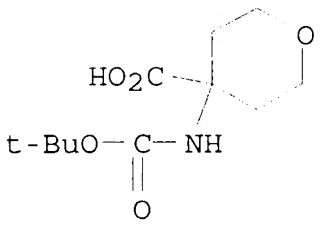
RN 150435-81-7 HCA
CN 4-Piperidinecarboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



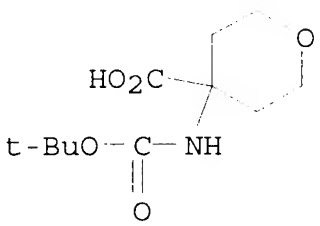
RN 162648-54-6 HCA
CN Cyclohexanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



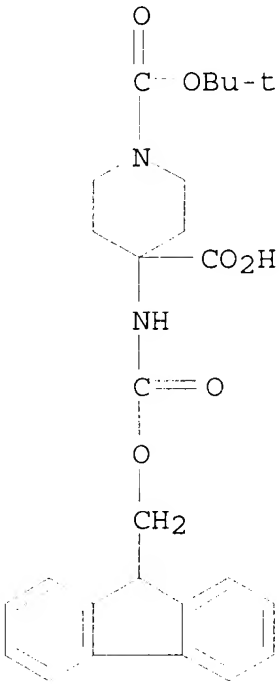
RN 172843-97-9 HCA
CN 2H-Pyran-4-carboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]tetrahydro- (9CI) (CA INDEX NAME)



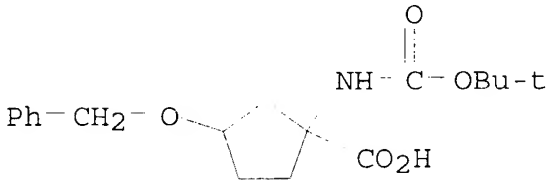
RN 172843-97-9 HCA
CN 2H-Pyran-4-carboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]tetrahydro- (9CI) (CA INDEX NAME)



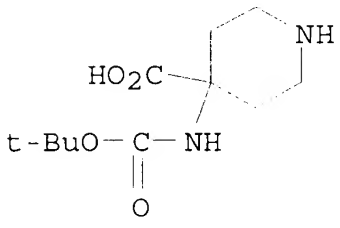
RN 183673-66-7 HCA
CN 1,4-Piperidinedicarboxylic acid, 4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



RN 191110-68-6 HCA
CN Cyclopentanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-(phenylmethoxy)- (9CI) (CA INDEX NAME)

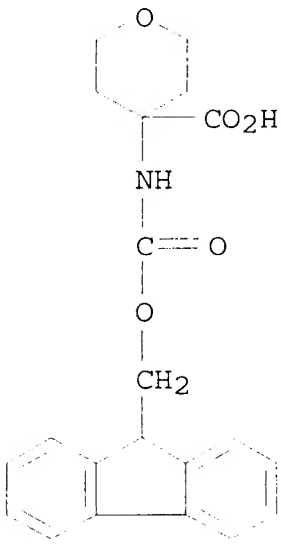


RN 252720-31-3 HCA
CN 4-Piperidinecarboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

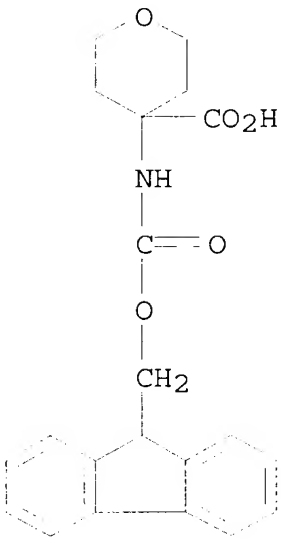


RN 285996-72-7 HCA
CN 2H-Pyran-4-carboxylic acid, 4-[[(9H-fluoren-9-

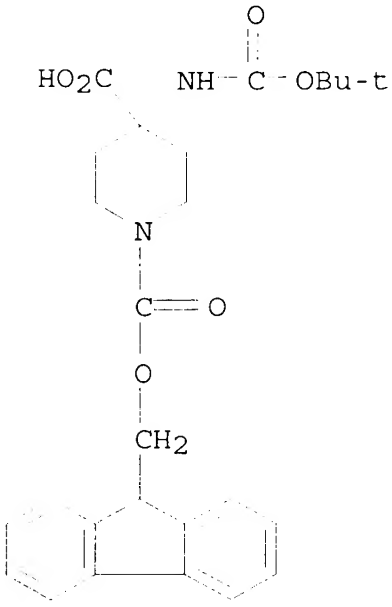
ylmethoxy)carbonyl]amino]tetrahydro- (9CI) (CA INDEX NAME)



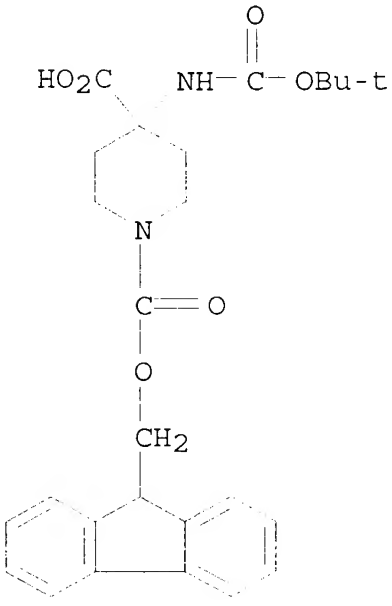
RN 285996-72-7 HCA
CN 2H-Pyran-4-carboxylic acid, 4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]tetrahydro- (9CI) (CA INDEX NAME)



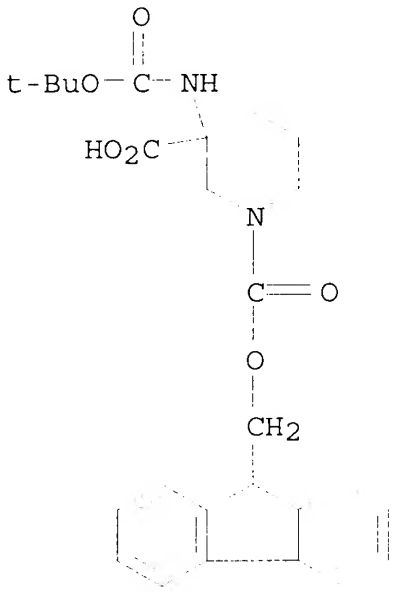
RN 368866-07-3 HCA
CN 1,4-Piperidinedicarboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-, 1-(9H-fluoren-9-ylmethyl) ester (9CI) (CA INDEX NAME)



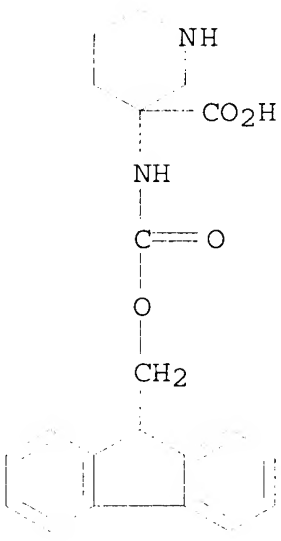
RN 368866-07-3 HCA
CN 1,4-Piperidinedicarboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-, 1-(9H-fluoren-9-ylmethyl) ester (9CI) (CA INDEX NAME)



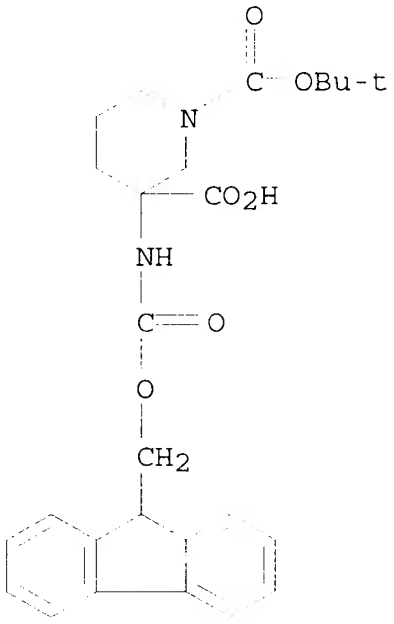
RN 368866-19-7 HCA
CN 1,3-Piperidinedicarboxylic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-, 1-(9H-fluoren-9-ylmethyl) ester (9CI) (CA INDEX NAME)



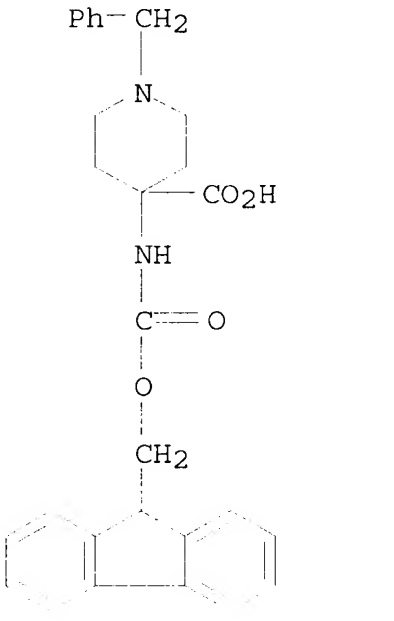
RN 368866-20-0 HCA
CN 3-Piperidinecarboxylic acid, 3-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



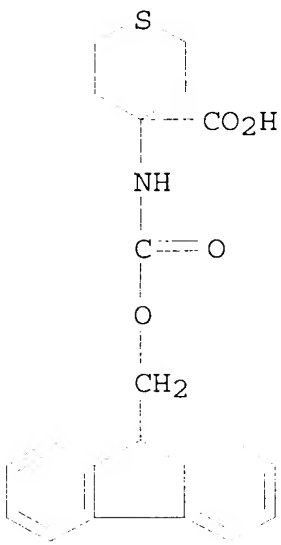
RN 368866-21-1 HCA
CN 1,3-Piperidinedicarboxylic acid, 3-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



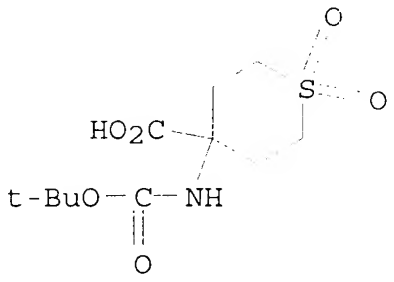
RN 368866-30-2 HCA
CN 4-Piperidinecarboxylic acid, 4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



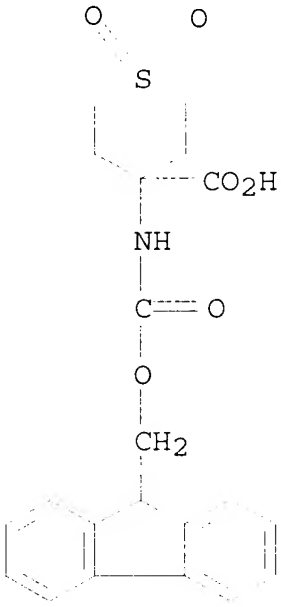
RN 368866-35-7 HCA
CN 2H-Thiopyran-4-carboxylic acid, 4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]tetrahydro- (9CI) (CA INDEX NAME)



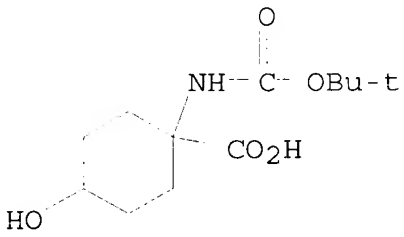
RN 369402-94-8 HCA
CN 2H-Thiopyran-4-carboxylic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]tetrahydro-, 1,1-dioxide (9CI) (CA INDEX NAME)



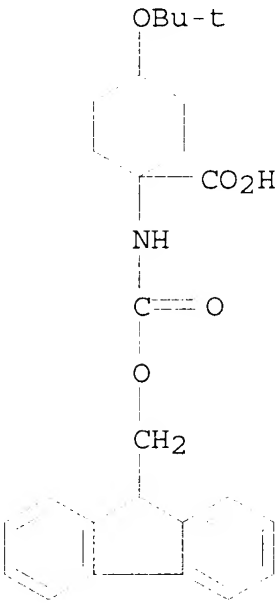
RN 369402-96-0 HCA
CN 2H-Thiopyran-4-carboxylic acid, 4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]tetrahydro-, 1,1-dioxide (9CI) (CA INDEX NAME)



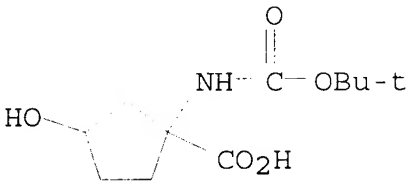
RN 369403-08-7 HCA
CN Cyclohexanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-4-hydroxy- (9CI) (CA INDEX NAME)



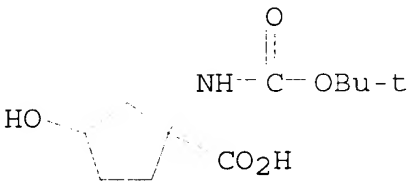
RN 369403-10-1 HCA
CN Cyclohexanecarboxylic acid, 4-(1,1-dimethylethoxy)-1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



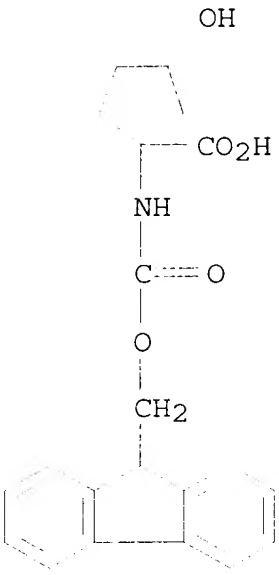
RN 369403-15-6 HCA
CN Cyclopentanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-hydroxy- (9CI) (CA INDEX NAME)



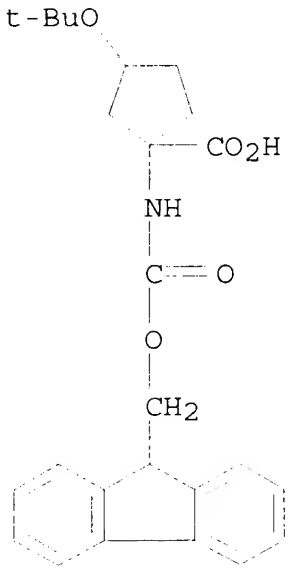
RN 369403-15-6 HCA
CN Cyclopentanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-hydroxy- (9CI) (CA INDEX NAME)



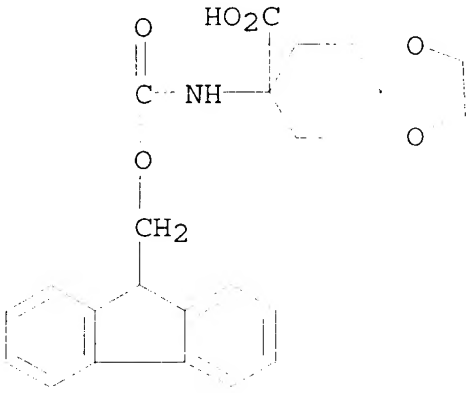
RN 369403-17-8 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-hydroxy- (9CI) (CA INDEX NAME)



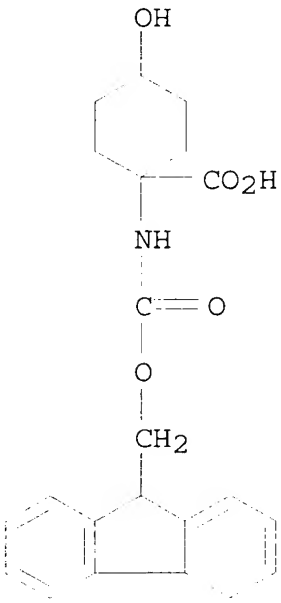
RN 369403-19-0 HCA
CN Cyclopentanecarboxylic acid, 3-(1,1-dimethylethoxy)-1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



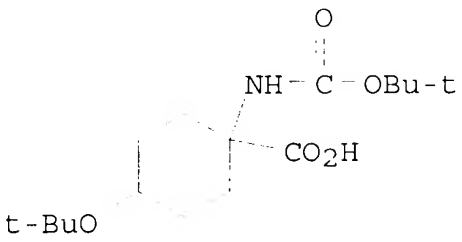
RN 369403-24-7 HCA
CN 1,4-Dioxaspiro[4.5]decane-8-carboxylic acid, 8-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



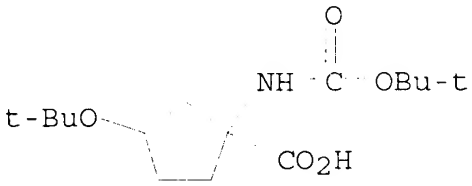
RN 436867-66-2 HCA
CN Cyclohexanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-4-hydroxy- (9CI) (CA INDEX NAME)



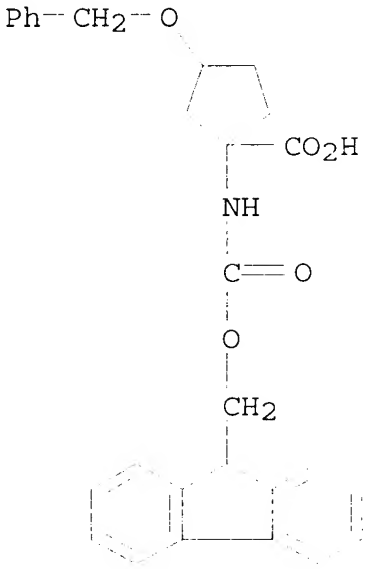
RN 436867-67-3 HCA
CN Cyclohexanecarboxylic acid, 4-(1,1-dimethylethoxy)-1-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



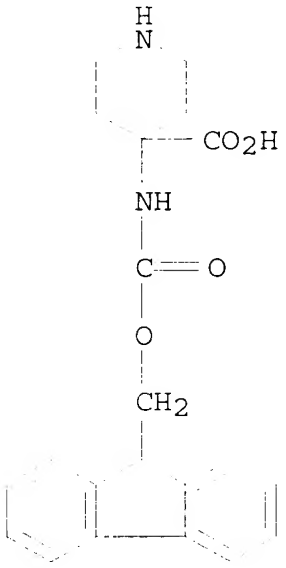
RN 436867-68-4 HCA
CN Cyclopentanecarboxylic acid, 3-(1,1-dimethylethoxy)-1-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



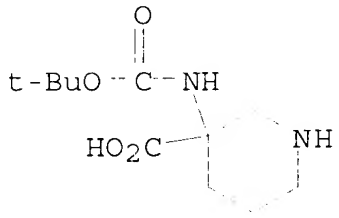
RN 436867-69-5 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-3-(phenylmethoxy)- (9CI) (CA INDEX NAME)



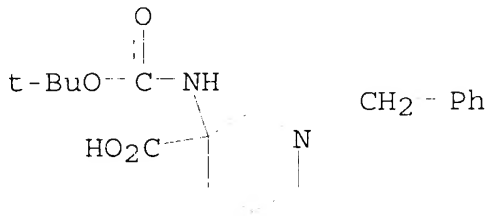
RN 436867-70-8 HCA
CN 4-Piperidinecarboxylic acid, 4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



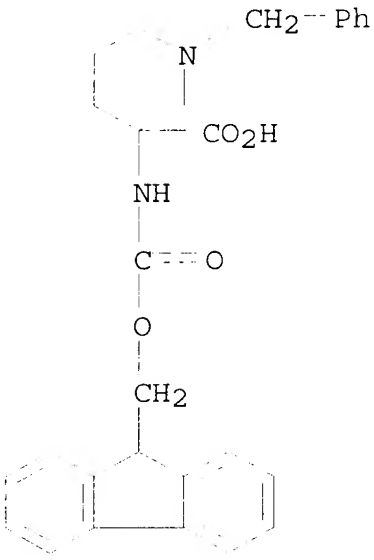
RN 436867-71-9 HCA
CN 3-Piperidinecarboxylic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 436867-72-0 HCA
CN 3-Piperidinecarboxylic acid, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 436867-73-1 HCA
CN 3-Piperidinecarboxylic acid, 3-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



IC ICM C07B061-00
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 24, 34
ST resin bound cyclic quaternary amino acid prepn combinatorial reagent; **Merrifield Wang** resin bound cyclic quaternary amino acid prepn
IT 7188-38-7, tert-Butyl isocyanide 19398-47-1, 1,4-Dibromo-2-butanol 29943-42-8, Tetrahydro-4-pyranone 41979-39-9, 4-Piperidone hydrochloride 69555-14-2, N-(Diphenylmethylene)glycine ethyl ester **217299-03-1**
(prepn. of resin-bound cyclic quaternary amino acids)
IT 13625-39-3P, 1,3,8-Triazaspiro[4.5]decane-2,4-dione 26562-23-2P **39124-20-4P** 183673-68-9P **252720-31-3P** **369403-17-8P** **369403-21-4P** **436867-74-2P** **436867-75-3P**
(prepn. of resin-bound cyclic quaternary amino acids)
IT **108329-81-3DP**, **Wang** and **Merrifield** resin-bound **150435-81-7DP**, **Wang** and **Merrifield** resin-bound **162648-54-6DP**, **Wang** and **Merrifield** resin-bound **172843-97-9DP**, **Wang** and **Merrifield** resin-bound **172843-97-9P** **183673-66-7DP**, **Wang** and **Merrifield** resin-bound **191110-68-6DP**, **Wang** and **Merrifield** resin-bound **252720-31-3DP**, **Wang** and **Merrifield** resin-bound **285996-72-7DP**, **Wang** and **Merrifield** resin-bound **285996-72-7P** **368866-07-3DP**, **Wang** and **Merrifield** resin-bound **368866-07-3P** **368866-19-7DP**, **Wang** and **Merrifield** resin-bound **368866-20-0DP**, **Wang** and **Merrifield** resin-bound **368866-21-1DP**,

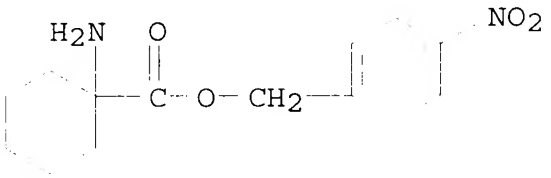
Wang and **Merrifield** resin-bound **368866-30-2DP**, **Wang** and **Merrifield** resin-bound **368866-35-7DP**, **Wang** and **Merrifield** resin-bound **369402-94-8DP**, **Wang** and **Merrifield** resin-bound **369402-96-0DP**, **Wang** and **Merrifield** resin-bound **369403-08-7DP**, **Wang** and **Merrifield** resin-bound **369403-10-1DP**, **Wang** and **Merrifield** resin-bound **369403-15-6DP**, **Wang** and **Merrifield** resin-bound **369403-15-6P** **369403-17-8DP**, **Wang** and **Merrifield** resin-bound **369403-19-0DP**, **Wang** and **Merrifield** resin-bound **369403-24-7DP**, **Wang** and **Merrifield** resin-bound **436867-66-2DP**, **Wang** and **Merrifield** resin-bound **436867-67-3DP**, **Wang** and **Merrifield** resin-bound **436867-68-4DP**, **Wang** and **Merrifield** resin-bound **436867-69-5DP**, **Wang** and **Merrifield** resin-bound **436867-70-8DP**, **Wang** and **Merrifield** resin-bound **436867-71-9DP**, **Wang** and **Merrifield** resin-bound **436867-72-0DP**, **Wang** and **Merrifield** resin-bound **436867-73-1DP**, **Wang** and **Merrifield** resin-bound
(prepn. of resin-bound cyclic quaternary amino acids)

L27 ANSWER 2 OF 16 HCA COPYRIGHT 2003 ACS

135:303848 2,6-Diketopiperazines from Amino Acids, from Solution-Phase to Solid-Phase Organic Synthesis. Perrotta, Enzo; Altamura, Maria; Barani, Teresa; Bindi, Simona; Giannotti, Danilo; Harmat, Nicholas J. S.; Nannicini, Rossano; Maggi, Carlo Alberto (Department of Chemistry, Menarini Ricerche S.p.A., Florence, I-50131, Italy). Journal of Combinatorial Chemistry, 3(5), 453-460 (English) 2001. CODEN: JCCHFF. ISSN: 1520-4766. Publisher: American Chemical Society.

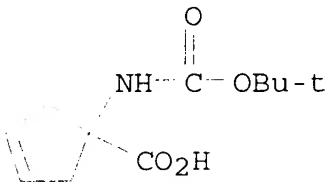
AB A method to prep. 1,3-disubstituted 2,6-diketopiperazines as useful heterocyclic library scaffolds in the search of new leads for drug discovery is described. The method can be used in soln.-phase and solid-phase conditions. In the key step of the synthesis, the imido portion of the new mol. is formed in soln. through intramol. cyclization, under basic conditions, of a secondary amide nitrogen on a benzyl ester. A **Wang** resin carboxylic ester is used as the acylating agent under solid-phase conditions, allowing the cyclization to take place with simultaneous cleavage of the product from the resin (cyclocleavage). The synthetic method worked well with several couples of amino acids, independently from their configuration, and was used for the parallel synthesis of a series of fully characterized compds. The use of iterative conditions in the solid phase (repeated addn. of fresh solvent and potassium carbonate to the resin after filtering out the product-contg. soln.) allowed the diastereoisomer content to be kept below the detection limit by HPLC and 1H NMR (200 MHz).

IT **366817-05-2**
(solid-phase and soln. synthesis of piperazinediones from amino acids)
RN 366817-05-2 HCA
CN Cyclohexanecarboxylic acid, 1-amino-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

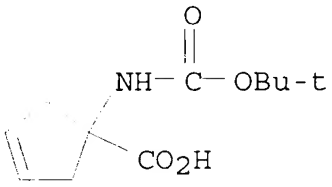


CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 34
IT 2577-90-4 4299-70-1 7352-64-9 13139-14-5, N-tert.-Butoxycarbonyl-L-tryptophan 16874-09-2 16874-17-2 21685-51-8 21691-50-9 21691-57-6 48067-24-9 57177-83-0 59624-87-2 63628-63-7 80165-23-7 366816-99-1 366817-02-9
366817-05-2 366817-07-4
(solid-phase and soln. synthesis of piperazinediones from amino acids)

L27 ANSWER 3 OF 16 HCA COPYRIGHT 2003 ACS
134:295776 Preparation of a 990-Member Chemical Compound Library of Hydantoin- and Isoxazoline-Containing Heterocycles Using Multipin Technology. Park, Kyung-Ho; Ehrler, Juerg; Spoerri, Heinz; Kurth, Mark J. (Department of Chemistry, University of California, Davis, CA, 95616, USA). Journal of Combinatorial Chemistry, 3(2), 171-176 (English) 2001. CODEN: JCCHFF. ISSN: 1520-4766. OTHER SOURCES: CASREACT 134:295776. Publisher: American Chemical Society.
AB The development of a useful chem. for the construction of polyfunctional heterocycles - first through soln. and solid phase (resins) and then library prodn. via SynPhase crowns - is reported. Bead-based synthetic work was done on **Merrifield** resin where treatment with benzylamine in the presence of DBU followed by reaction with 4-chloromethylbenzoyl chloride afforded an amide-linked resin. Finally, TFA.cntdot.NH2-polystyrene macro crowns were derivatized with 4-(hydroxymethyl)benzoic acid to afford pin, which was coupled with a Boc-protected amino acid in the presence of DIC to deliver pin.
IT **213316-20-2 334709-11-4**
(prepn. of a library of hydantoin- and isoxazoline-contg. heterocycles using multipin technol.)
RN 213316-20-2 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

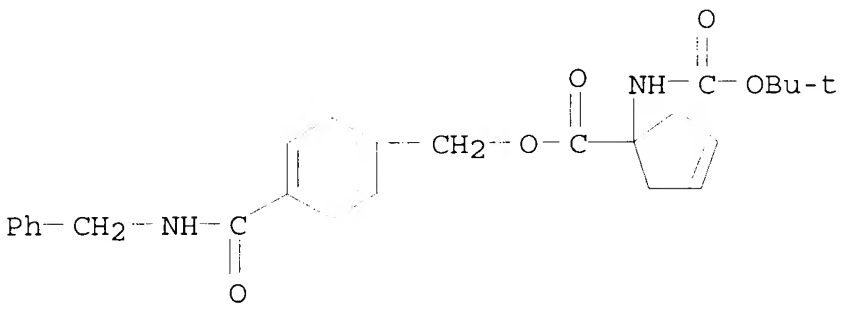


RN 334709-11-4 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-, monopotassium salt (9CI) (CA INDEX NAME)

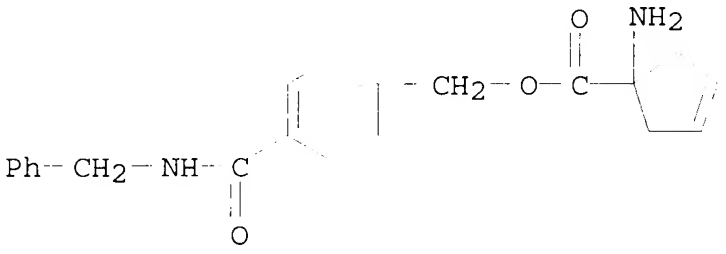


● K

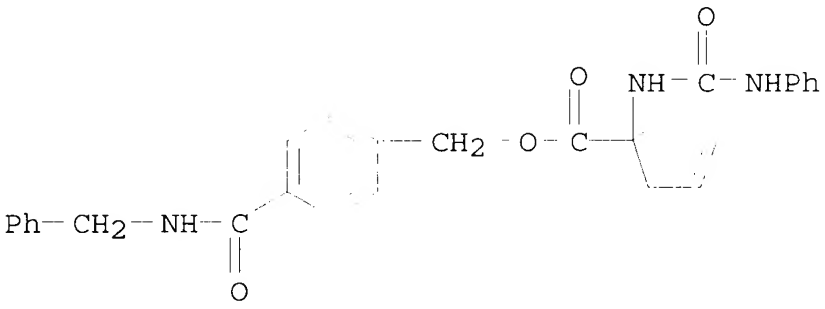
IT **334709-07-8P 334709-08-9P 334709-09-0P**
334709-10-3P
(prepn. of a library of hydantoin- and isoxazoline-contg. heterocycles using multipin technol.)
RN 334709-07-8 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-, [4-[[(phenylmethyl)amino]carbonyl]phenyl]methyl ester (9CI) (CA INDEX NAME)



RN 334709-08-9 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-amino-, [4-[[(phenylmethyl)amino]carbonyl]phenyl]methyl ester (9CI) (CA INDEX NAME)

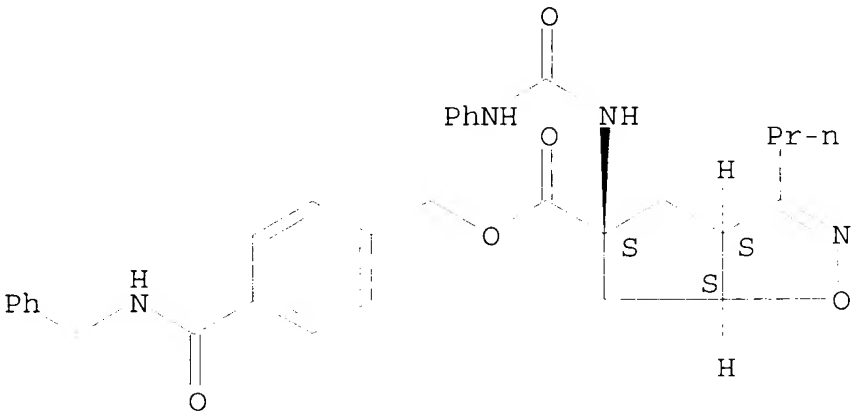


RN 334709-09-0 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[(phenylamino)carbonyl]amino]-, [4-[[(phenylmethyl)amino]carbonyl]phenyl]methyl ester (9CI) (CA INDEX NAME)



RN 334709-10-3 HCA
CN 4H-Cyclopent[d]isoxazole-5-carboxylic acid, 3a,5,6,6a-tetrahydro-5-[[(phenylamino)carbonyl]amino]-3-propyl-, [4-[[(phenylmethyl)amino]carbonyl]phenyl]methyl ester, (3aR,5R,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 100-46-9, Benzylamine, reactions 103-71-9, Phenyl isocyanate, reactions 108-03-2, 1-Nitropropane 627-05-4, 1-Nitrobutane 876-08-4, 4-Chloromethylbenzoyl chloride 3006-96-0, 4-(Hydroxymethyl)benzoic acid **213316-20-2** 334709-06-7 **334709-11-4**
(prepn. of a library of hydantoin- and isoxazoline-contg. heterocycles using multipin technol.)

IT **334709-07-8P 334709-08-9P 334709-09-0P 334709-10-3P**
(prepn. of a library of hydantoin- and isoxazoline-contg. heterocycles using multipin technol.)

L27 ANSWER 4 OF 16 HCA COPYRIGHT 2003 ACS

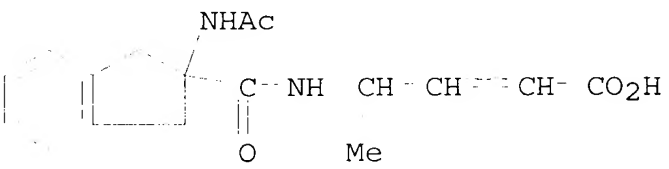
134:71867 Parallel solid-phase synthesis of peptidyl Michael acceptors. Caulfield, Thomas J.; Patel, Sharmila; Salvino, Joseph M.; Liester, Lara; Labaudiniere, Richard (Lead Discovery Department, Rhone-Poulenc Rorer, Collegeville, PA, USA). Journal of Combinatorial Chemistry, 2(6), 600-603 (English) 2000. CODEN: JCCHFF. ISSN: 1520-4766. OTHER SOURCES: CASREACT 134:71867. Publisher: American Chemical Society.

AB A general solid-phase approach for the efficient parallel synthesis of peptidyl Michael acceptors has been developed. This method furnished a no. of potential inhibitors of cysteine protease. This approach featured the efficient synthesis of peptide aldehydes in parallel from resin-bound Weinreb amides. These were obtained from readily available Fmoc-amino acids and N-benzyl **Wang** -O-hydroxylamine resin. The resin-bound Weinreb amides allowed for the parallel generation of N-protected amino aldehydes on solid-phase, which offered several advantages over soln.-phase synthesis. For example, a wide variety of amino aldehydes can be generated from any carboxylic acid; the synthesis allows for the facile generation of a diverse no. of products in parallel over a no. of synthetic steps without laborious extractive workup procedures and chromatog. purifications. These N-protected amino aldehydes were, next, used in a supported Horner-Emmons reaction, the key step, to generate various Michael acceptors, which were finally cleaved from the resin using 50% TFA. Overall, using this approach worked very well to rapidly survey the initial chem. on resin on a 20 mg to 1g scale.

IT **315667-59-5P**
(parallel solid-phase synthesis of peptidyl Michael acceptors from Weinreb amide precursors)

RN 315667-59-5 HCA

CN 2-Pentenoic acid, 4-[[[2-(acetylamino)-2,3-dihydro-1H-inden-2-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)



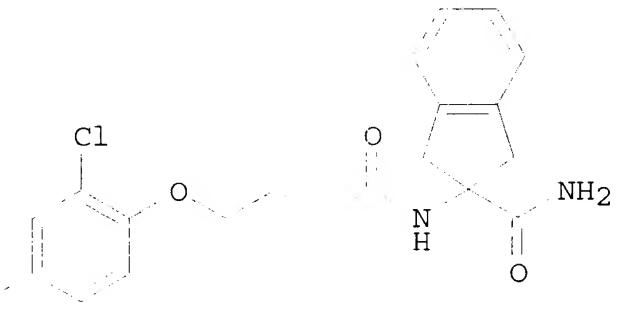
CC 34-3 (Amino Acids, Peptides, and Proteins)

IT 315667-17-5P 315667-18-6P 315667-19-7P 315667-20-0P
315667-26-6P 315667-27-7P 315667-28-8P 315667-29-9P
315667-38-0P 315667-39-1P 315667-40-4P 315667-41-5P
315667-46-0P 315667-47-1P 315667-48-2P 315667-49-3P
315667-50-6P 315667-51-7P 315667-52-8P 315667-53-9P
315667-54-0P 315667-55-1P 315667-56-2P 315667-57-3P
315667-58-4P **315667-59-5P** 315667-60-8P 315667-61-9P
315667-62-0P 315667-63-1P 315667-64-2P 315667-65-3P
315667-66-4P 315667-67-5P 315667-68-6P 315667-69-7P
315667-70-0P 315667-71-1P 315667-72-2P 315667-73-3P
315667-74-4P 315667-75-5P 315667-76-6P 315667-77-7P
315667-78-8P
(parallel solid-phase synthesis of peptidyl Michael acceptors from Weinreb amide precursors)

L27 ANSWER 5 OF 16 HCA COPYRIGHT 2003 ACS

129:331032 Exploring structure-activity relationships around the phosphomannose isomerase inhibitor AF14049 via combinatorial synthesis. Bhandari, Ashok; Jones, David G.; Schullek, John R.; Vo, Kham; Schunk, Caryn A.; Tamanaha, Lisa L.; Chen, Dawn; Yuan, Zhengyu; Needels, Michael C.; Gallop, Mark A. (Affymax Research Institute, Palo Alto, CA, 94304, USA). Bioorganic & Medicinal Chemistry Letters, 8(17), 2303-2308 (English) 1998. CODEN: BMCLE8. ISSN: 0960-894X. Publisher: Elsevier Science Ltd..

GI

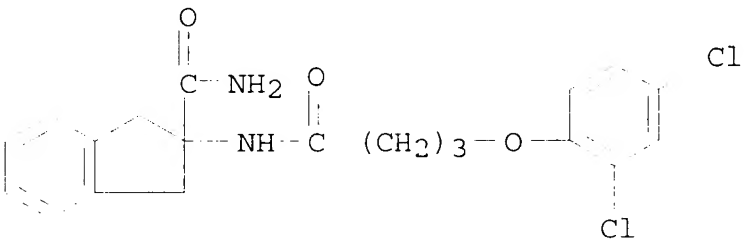


I

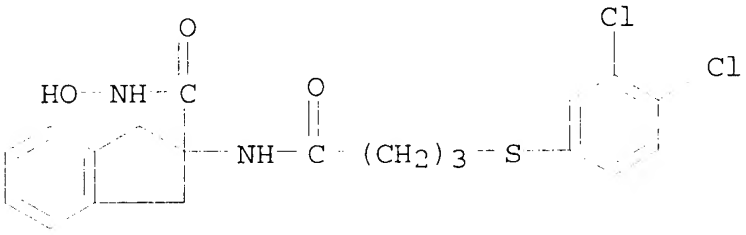
AB Phosphomannose isomerase (PMI) has been shown by genetic methods to be an essential enzyme in fungal cell wall biosynthesis. The PMI inhibitor AF14049 (I) was discovered as an unanticipated side product from high-throughput library screening against the enzyme from C. albicans. **Solid-phase synthetic** methods were developed and a series of libraries and discrete analogs synthesized to explore SAR around AF14049.

IT **215313-40-9**, AF 14049 **215313-41-0**, AF 15394
(structure-activity of aminoindanecarboxamide phosphomannose isomerase inhibitor AF14049 via combinatorial synthesis)

RN 215313-40-9 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)

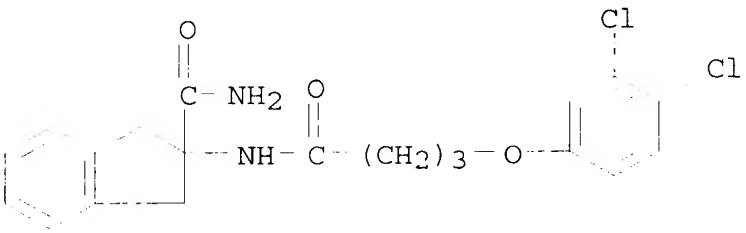


RN 215313-41-0 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-[(3,4-dichlorophenyl)thio]-1-oxobutyl]amino]-2,3-dihydro-N-hydroxy- (9CI) (CA INDEX NAME)

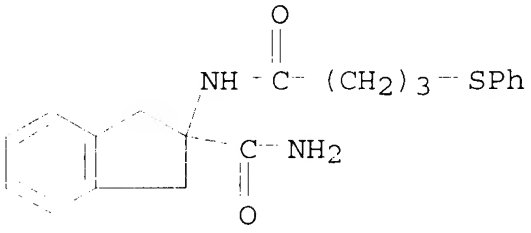


IT **215094-86-3P 215094-87-4DP**, combinatorial library derivs. **215094-89-6P 215094-90-9DP**, combinatorial library derivs. **215094-91-0P 215094-92-1P 215094-93-2P 215094-94-3DP**, combinatorial library reaction products with (arylthio)- and (arylamino)alkanoic acids **215094-95-4P 215094-96-5P 215094-99-8P 215095-00-4P 215095-02-6P 215095-03-7P 215095-04-8P 215095-05-9P 215095-06-0P 215095-07-1P 215095-08-2P 215095-09-3P 215095-10-6DP**, combinatorial library derivs. **215095-11-7P**
(structure-activity of aminoindanecarboxamide phosphomannose isomerase inhibitor AF14049 via combinatorial synthesis)

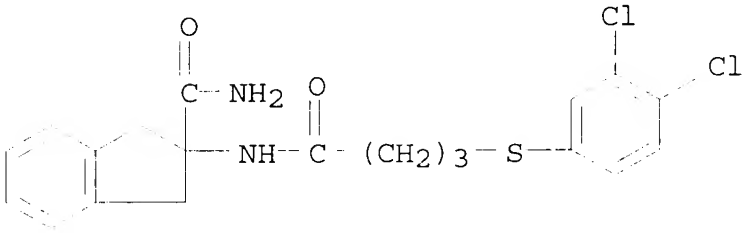
RN 215094-86-3 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-(3,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



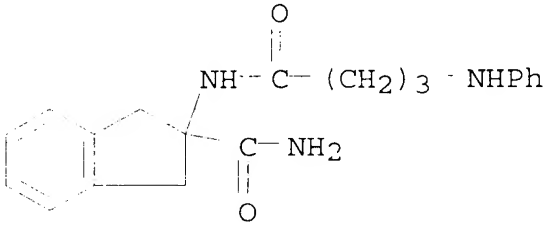
RN 215094-87-4 HCA
CN 1H-Indene-2-carboxamide, 2,3-dihydro-2-[[1-oxo-4-(phenylthio)butyl]amino]- (9CI) (CA INDEX NAME)



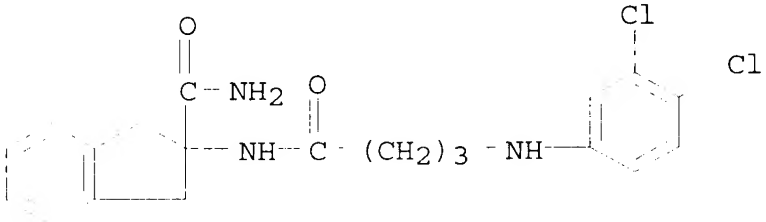
RN 215094-89-6 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-[(3,4-dichlorophenyl)thio]-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



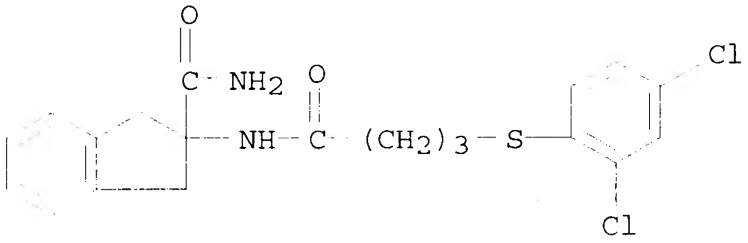
RN 215094-90-9 HCA
CN 1H-Indene-2-carboxamide, 2,3-dihydro-2-[[1-oxo-4-(phenylamino)butyl]amino]- (9CI) (CA INDEX NAME)



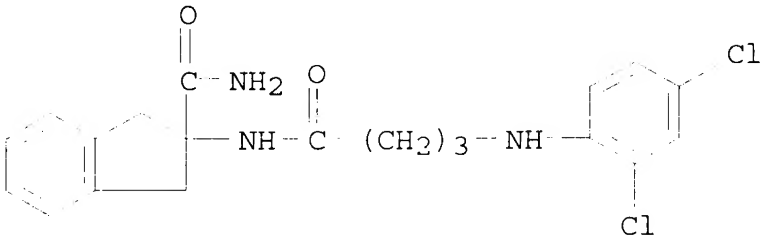
RN 215094-91-0 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-[(3,4-dichlorophenyl)amino]-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



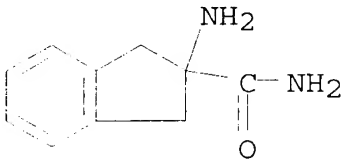
RN 215094-92-1 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-[(2,4-dichlorophenyl)thio]-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



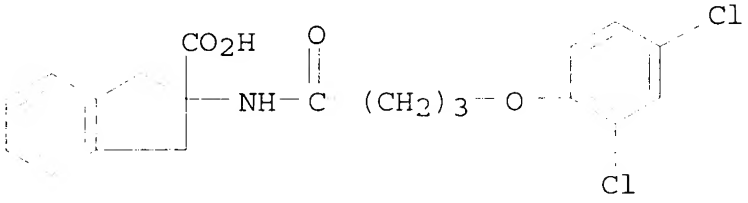
RN 215094-93-2 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-[(2,4-dichlorophenyl)amino]-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



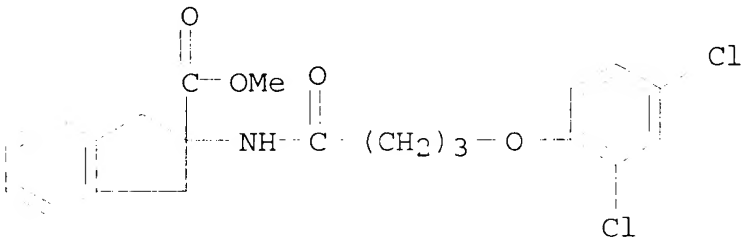
RN 215094-94-3 HCA
CN 1H-Indene-2-carboxamide, 2-amino-2,3-dihydro- (9CI) (CA INDEX NAME)



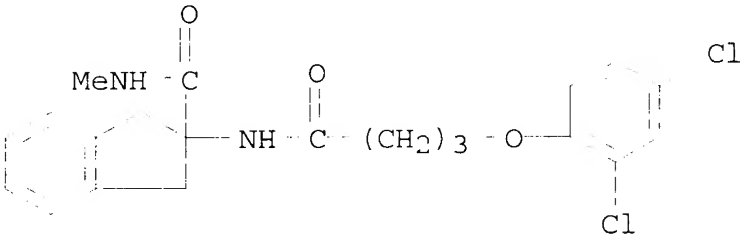
RN 215094-95-4 HCA
CN 1H-Indene-2-carboxylic acid, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



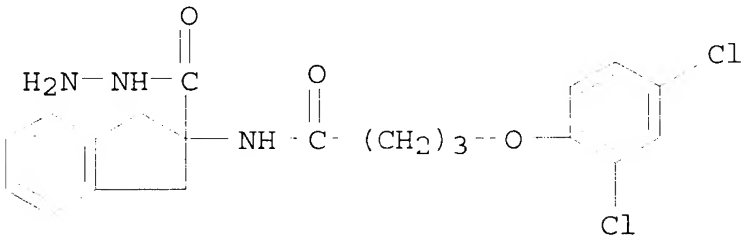
RN 215094-96-5 HCA
CN 1H-Indene-2-carboxylic acid, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro-, methyl ester (9CI) (CA INDEX NAME)



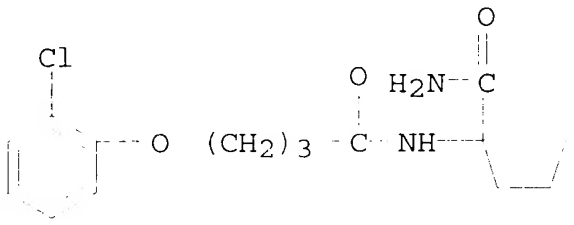
RN 215094-99-8 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro-N-methyl- (9CI) (CA INDEX NAME)



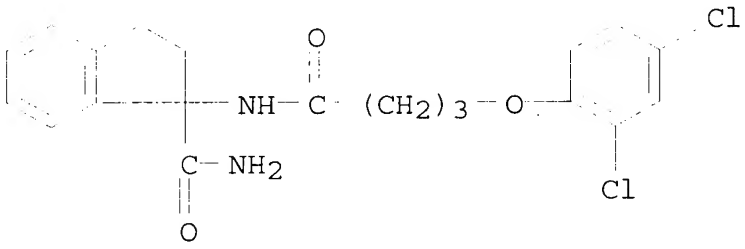
RN 215095-00-4 HCA
CN 1H-Indene-2-carboxylic acid, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro-, hydrazide (9CI) (CA INDEX NAME)



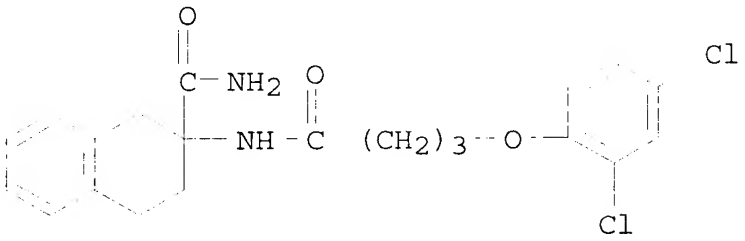
RN 215095-02-6 HCA
CN Cyclopentanecarboxamide, 1-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]- (9CI) (CA INDEX NAME)



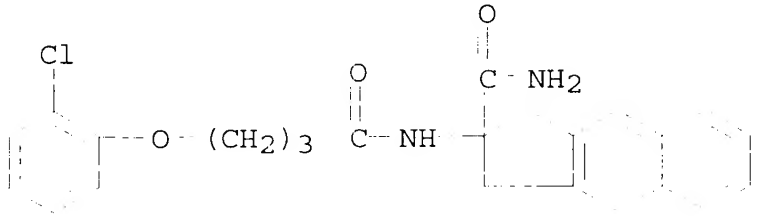
RN 215095-03-7 HCA
CN 1H-Indene-1-carboxamide, 1-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



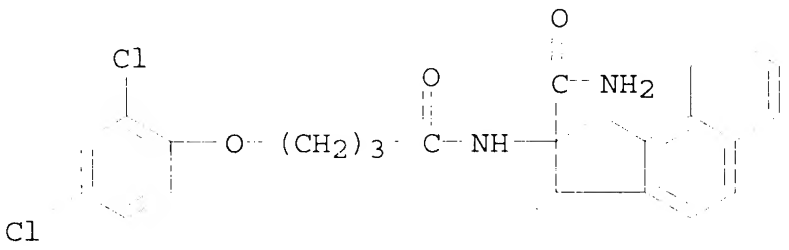
RN 215095-04-8 HCA
CN 2-Naphthalenecarboxamide, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)



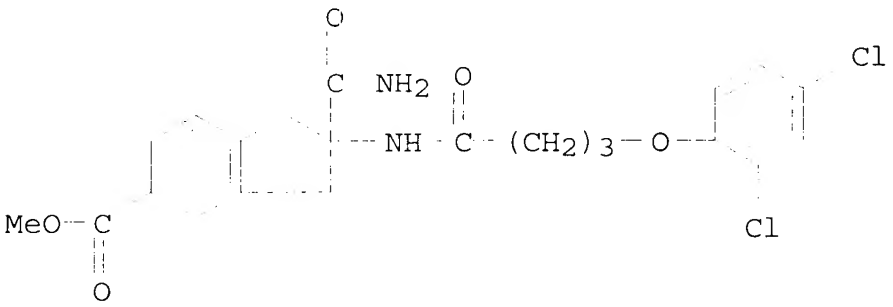
RN 215095-05-9 HCA
CN 1H-Benz[f]indene-2-carboxamide, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



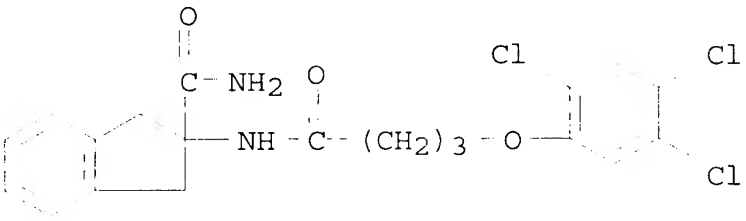
RN 215095-06-0 HCA
CN 1H-Benz[e]indene-2-carboxamide, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



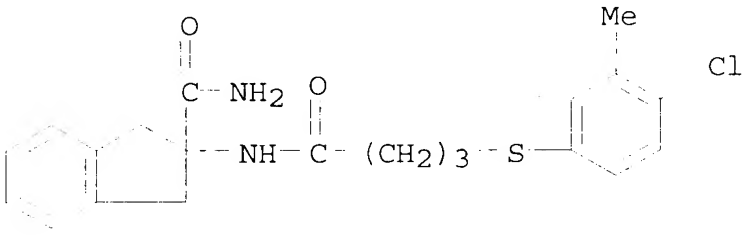
RN 215095-07-1 HCA
CN 1H-Indene-5-carboxylic acid, 2-(aminocarbonyl)-2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro-, methyl ester (9CI) (CA INDEX NAME)



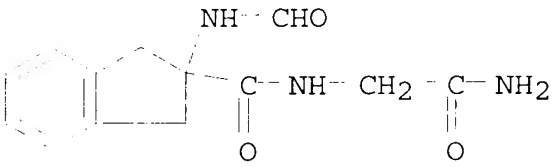
RN 215095-08-2 HCA
CN 1H-Indene-2-carboxamide, 2,3-dihydro-2-[[1-oxo-4-(2,4,5-trichlorophenoxy)butyl]amino]- (9CI) (CA INDEX NAME)



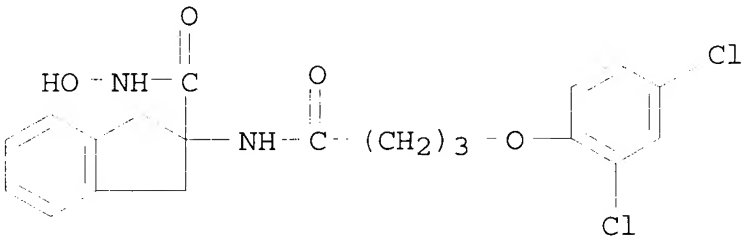
RN 215095-09-3 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-[(4-chloro-3-methylphenyl)thio]-1-oxobutyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)



RN 215095-10-6 HCA
CN 1H-Indene-2-carboxamide, N-(2-amino-2-oxoethyl)-2-(formylamino)-2,3-dihydro- (9CI) (CA INDEX NAME)



RN 215095-11-7 HCA
CN 1H-Indene-2-carboxamide, 2-[[4-(2,4-dichlorophenoxy)-1-oxobutyl]amino]-2,3-dihydro-N-hydroxy- (9CI) (CA INDEX NAME)



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 7, 10
IT **215313-40-9**, AF 14049 **215313-41-0**, AF 15394
(structure-activity of aminoindanecarboxamide phosphomannose isomerase inhibitor AF14049 via combinatorial synthesis)
IT **215094-86-3P 215094-87-4DP**, combinatorial library derivs. **215094-89-6P 215094-90-9DP**, combinatorial library derivs. **215094-91-0P** **215094-92-1P 215094-93-2P 215094-94-3DP**, combinatorial library reaction products with (arylthio)- and (arylamino)alkanoic acids **215094-95-4P** **215094-96-5P** 215094-97-6P 215094-98-7P **215094-99-8P 215095-00-4P** 215095-01-5P **215095-02-6P 215095-03-7P 215095-04-8P** **215095-05-9P 215095-06-0P 215095-07-1P** **215095-08-2P 215095-09-3P 215095-10-6DP**, combinatorial library derivs. **215095-11-7P** 215095-13-9P

(structure-activity of aminoindanecarboxamide phosphomannose isomerase inhibitor AF14049 via combinatorial synthesis)

L27 ANSWER 6 OF 16 HCA COPYRIGHT 2003 ACS

129:302872 Synthesis, biological activity, and conformational studies of insect allatostatin neuropeptide analogs incorporating turn-promoting moieties. Nachman, Ronald J.; Moyna, Guillermo; Williams, Howard J.; Tobe, Stephen S.; Scott, A. I. (Veterinary Entomology Research Unit, FAPRL, Agricultural Research Service, USDA, College Station, TX, 77845-2122, USA). Bioorganic & Medicinal Chemistry, 6(8), 1379-1388 (English) 1998. CODEN: BMECEP. ISSN: 0968-0896. Publisher: Elsevier Science Ltd..

AB Allatostatins are 6-18 residue peptides synthesized by insects to control prodn. of juvenile hormones, which in turn regulate functions including metamorphosis and egg prodn. Four insect allatostatin neuropeptide analogs incorporating turn-promoting pseudopeptide moieties in the region responsible for biol. activity were prepd. by **solid phase** peptide **synthetic** methods. Bioassay indicated that activities approached those of the natural neuropeptides, and mol. models based on NMR data showed similar conformations and the presence of a .beta.-turn in the active core region for the four analogs. Differences in activity are believed to be due to differences in bulk and relative position of atoms in the unnatural portion of the analogs, and their differing degrees of conformational freedom. The studies support the feasibility of development of neuropeptide-based insect control agents resistant to peptidase deactivation.

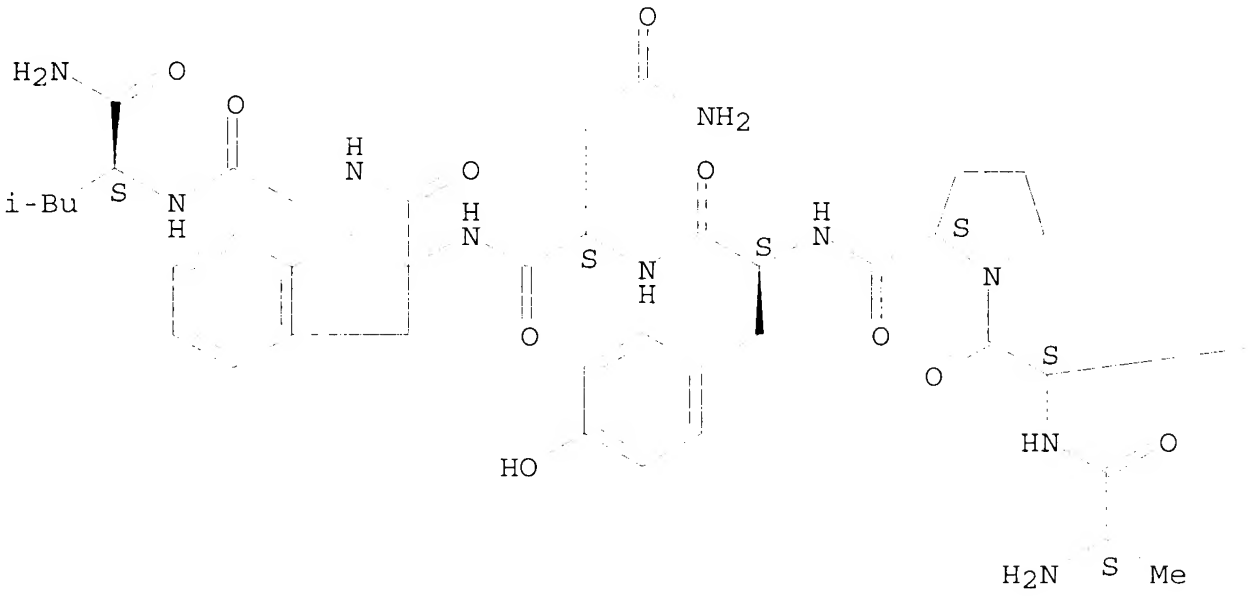
IT **214470-28-7P 214470-29-8P 214470-30-1P**
(prepn., biol. activity, and conformational studies of insect allatostatin neuropeptide analogs incorporating .beta.-turn-promoting moieties)

RN 214470-28-7 HCA

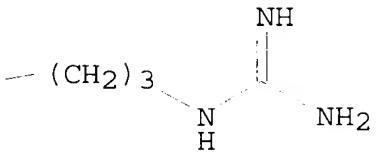
CN L-Leucinamide, L-alanyl-L-arginyl-L-prolyl-L-tyrosyl-L-asparaginyl-2-amino-2,3-dihydro-1H-indene-2-carbonylglycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



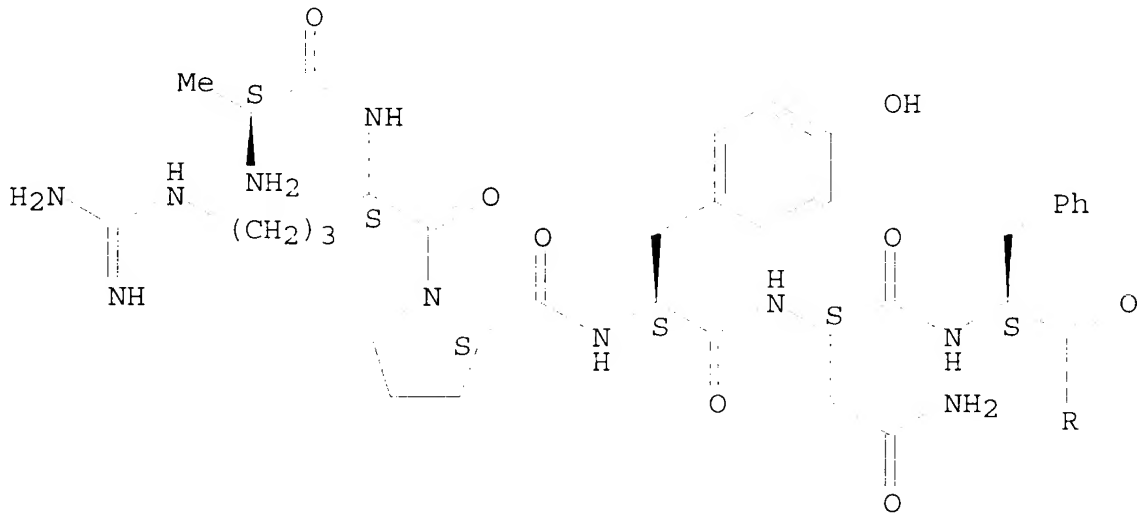
PAGE 1-B



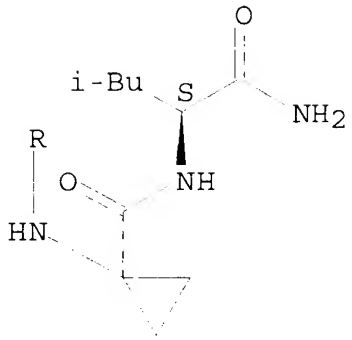
RN 214470-29-8 HCA
CN L-Leucinamide, L-alanyl-L-arginyl-L-prolyl-L-tyrosyl-L-asparaginyl-L-phenylalanyl-1-aminocyclopropanecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



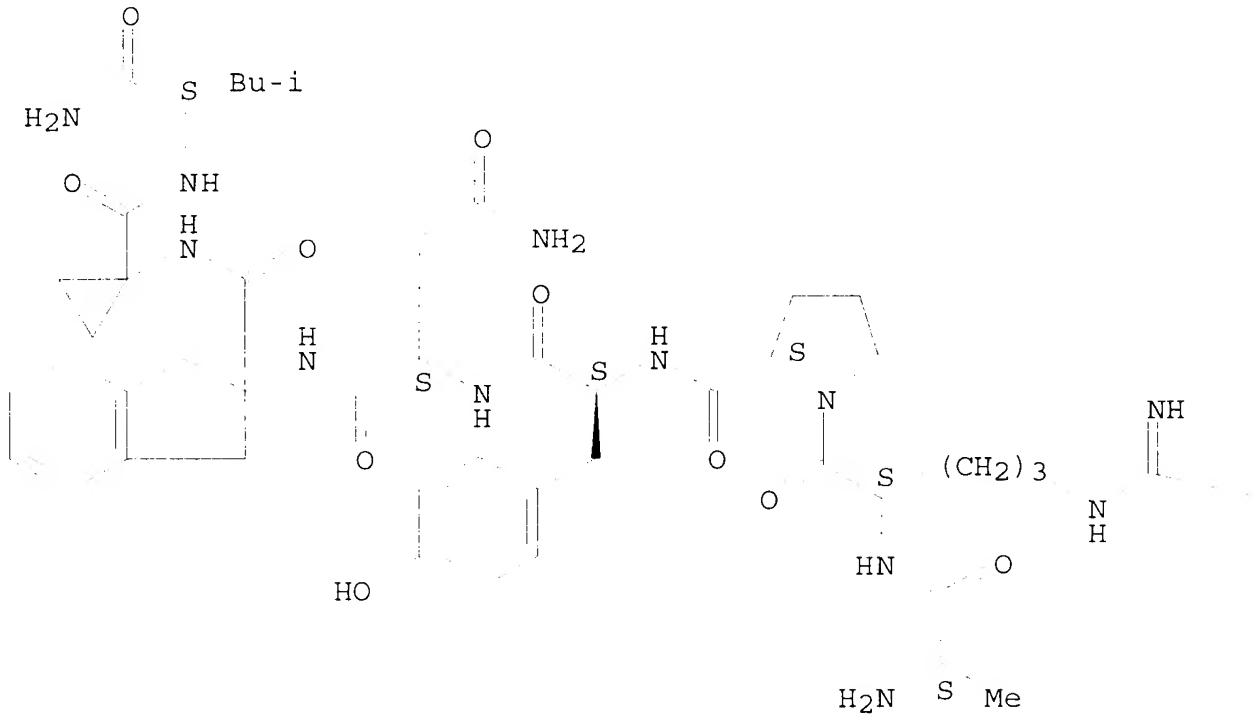
PAGE 2-A



RN 214470-30-1 HCA
CN L-Leucinamide, L-alanyl-L-arginyl-L-prolyl-L-tyrosyl-L-asparaginyl-2-amino-2,3-dihydro-1H-indene-2-carbonyl-1-aminocyclopropanecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 5, 12, 22

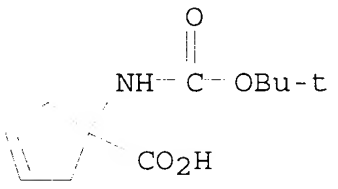
IT **214470-28-7P 214470-29-8P 214470-30-1P**
214470-31-2P 214470-32-3P
(prepn., biol. activity, and conformational studies of insect allatostatin neuropeptide analogs incorporating .beta.-turn-promoting moieties)

L27 ANSWER 7 OF 16 HCA COPYRIGHT 2003 ACS
129:245085 Diastereoselective Solid-Phase Synthesis of Novel Hydantoin- and Isoxazoline-Containing Heterocycles. Park, Kyung-Ho; Olmstead, Marilyn M.; Kurth, Mark J. (Department of Chemistry, University of California, Davis, CA, 95616, USA). Journal of Organic Chemistry, 63(19), 6579-6585 (English) 1998. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB Novel spirocyclic isoxazoloimidazolidinedione heterocycles were prepd. by exploiting 1,3-dipolar cycloaddn. and carbanilide cyclization transformations on solid phase starting from **Merrifield** resin. Cyclopentanoid isoxazoloimidazolidinediones were obtained with complete diastereoselectivity, and cyclopropanoid isoxazoloimidazolidinediones were obtained as an .apprxeq.2:1 mixt. of diastereomers.

IT **213316-20-2**
(stereoselective solid-phase synthesis of novel hydantoin- and isoxazoline-contg. spiro compds.)

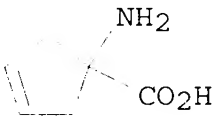
RN 213316-20-2 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



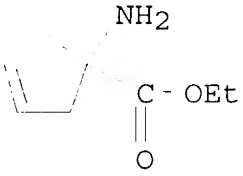
IT **27314-05-2DP**, polymer-bound **199532-88-2P**
207729-00-8P 210709-45-8DP, polymer-bound
213316-20-2DP, polymer-bound **213316-21-3DP**,
polymer-bound **213316-22-4DP**, polymer-bound
213316-23-5DP, polymer-bound **213316-24-6DP**,
polymer-bound **213316-25-7DP**, polymer-bound
213316-26-8DP, polymer-bound **213316-27-9DP**,
polymer-bound **213316-28-0DP**, polymer-bound
213316-32-6P 213316-34-8P 213316-35-9P
213316-36-0P 213316-37-1P 213316-38-2P
213316-39-3P 213316-49-5P 213316-50-8DP,
polymer-bound **213316-50-8P 213316-51-9DP**,
polymer-bound **213316-52-0DP**, polymer-bound
213316-53-1DP, polymer-bound **213316-54-2DP**,
polymer-bound **213316-56-4DP**, polymer-bound
213316-58-6DP, polymer-bound **213316-59-7DP**,

polymer-bound
(stereoselective solid-phase synthesis of novel hydantoin- and isoxazoline-contg. spiro compds.)

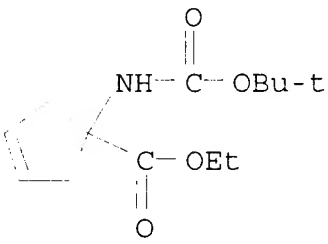
RN 27314-05-2 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-amino- (8CI, 9CI) (CA INDEX NAME)



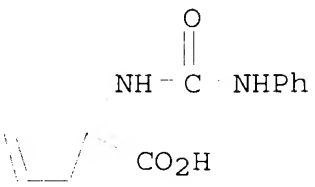
RN 199532-88-2 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-amino-, ethyl ester (9CI) (CA INDEX NAME)



RN 207729-00-8 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

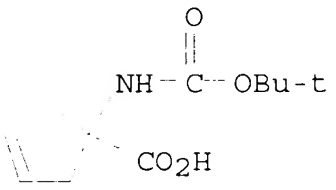


RN 210709-45-8 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)

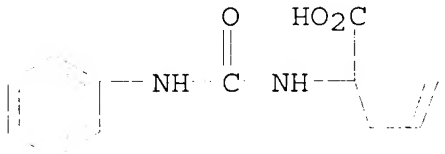


RN 213316-20-2 HCA

CN 3-Cyclopentene-1-carboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

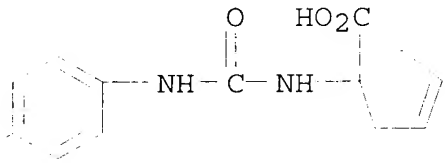


RN 213316-21-3 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[[(4-chlorophenyl)amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



Cl

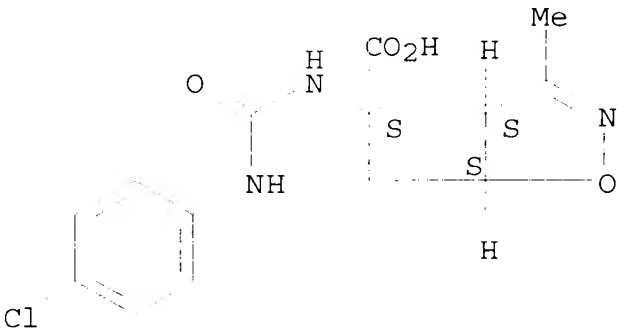
RN 213316-22-4 HCA
CN 3-Cyclopentene-1-carboxylic acid, 1-[[[(4-fluorophenyl)amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



F

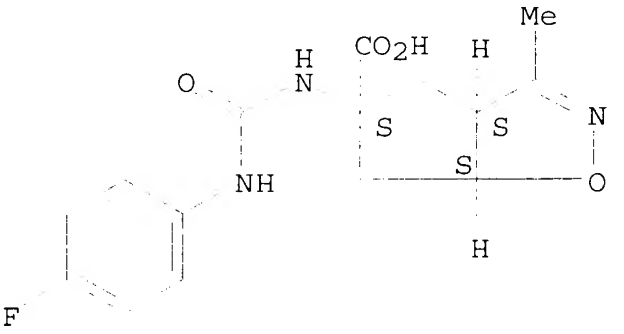
RN 213316-23-5 HCA
CN 4H-Cyclopent[d]isoxazole-5-carboxylic acid, 5-[[[(4-chlorophenyl)amino]carbonyl]amino]-3a,5,6,6a-tetrahydro-3-methyl-, (3aR,5R,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



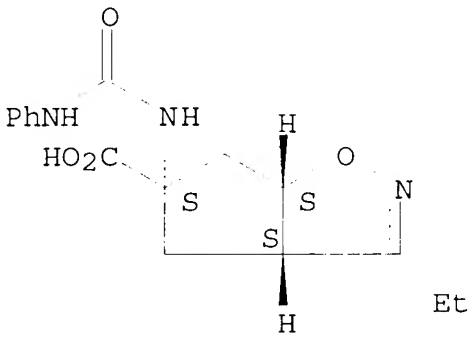
RN 213316-24-6 HCA
CN 4H-Cyclopent[d]isoxazole-5-carboxylic acid, 5-[[[(4-fluorophenyl)amino]carbonyl]amino]-3a,5,6,6a-tetrahydro-3-methyl-, (3aR,5R,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



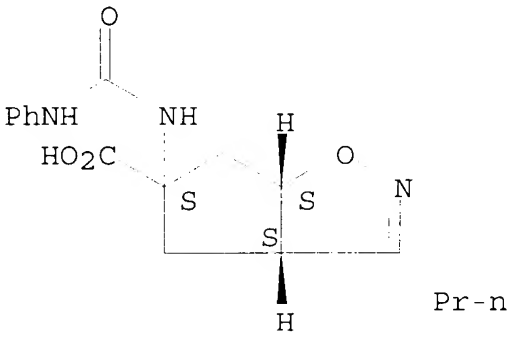
RN 213316-25-7 HCA
CN 4H-Cyclopent[d]isoxazole-5-carboxylic acid, 3-ethyl-3a,5,6,6a-tetrahydro-5-[[(phenylamino)carbonyl]amino]-, (3aR,5R,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



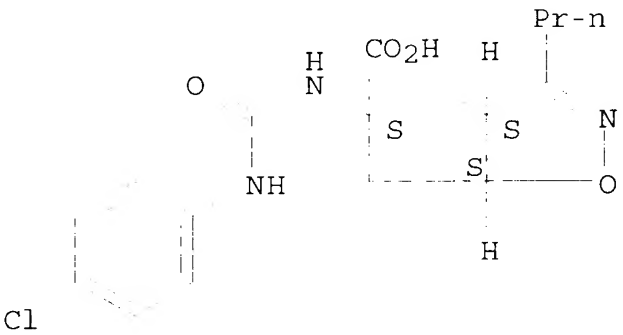
RN 213316-26-8 HCA
CN 4H-Cyclopent[d]isoxazole-5-carboxylic acid, 3a,5,6,6a-tetrahydro-5-[[(phenylamino)carbonyl]amino]-3-propyl-, (3aR,5R,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



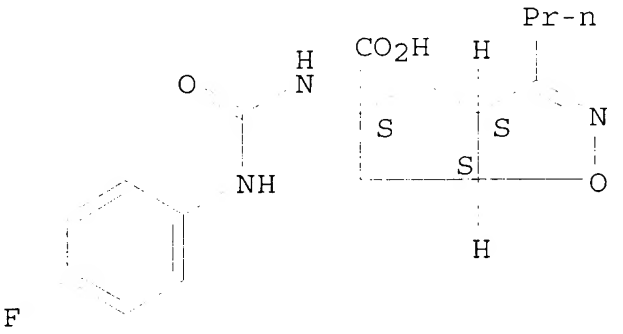
RN 213316-27-9 HCA
CN 4H-Cyclopent[d]isoxazole-5-carboxylic acid, 5-[[[(4-chlorophenyl)amino]carbonyl]amino]-3a,5,6,6a-tetrahydro-3-propyl-, (3aR,5R,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



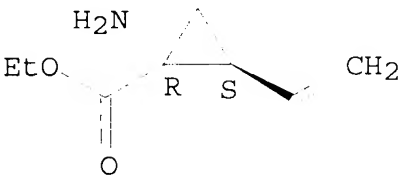
RN 213316-28-0 HCA
CN 4H-Cyclopent[d]isoxazole-5-carboxylic acid, 5-[[[(4-fluorophenyl)amino]carbonyl]amino]-3a,5,6,6a-tetrahydro-3-propyl-, (3aR,5R,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



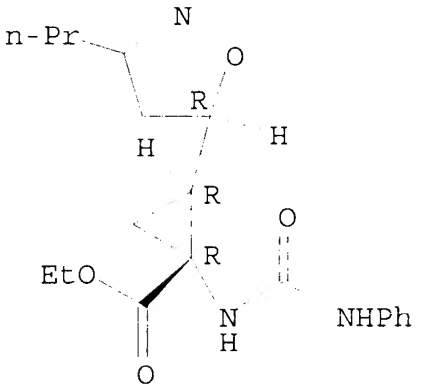
RN 213316-32-6 HCA
CN Cyclopropanecarboxylic acid, 1-amino-2-ethenyl-, ethyl ester, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



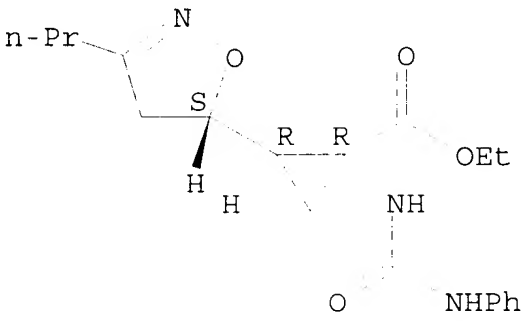
RN 213316-34-8 HCA
CN Cyclopropanecarboxylic acid, 2-[(5R)-4,5-dihydro-3-propyl-5-isoxazolyl]-1-[[(phenylamino)carbonyl]amino]-, ethyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



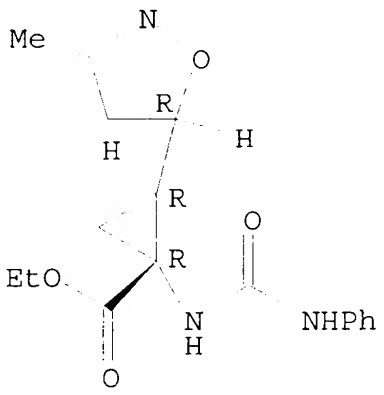
RN 213316-35-9 HCA
CN Cyclopropanecarboxylic acid, 2-[(5R)-4,5-dihydro-3-propyl-5-isoxazolyl]-1-[[(phenylamino)carbonyl]amino]-, ethyl ester, (1S,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



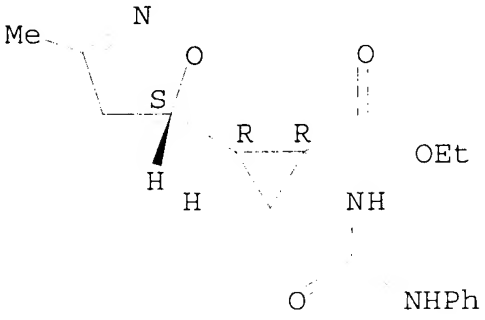
RN 213316-36-0 HCA
CN Cyclopropanecarboxylic acid, 2-[(5R)-4,5-dihydro-3-methyl-5-isoxazolyl]-1-[[(phenylamino)carbonyl]amino]-, ethyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



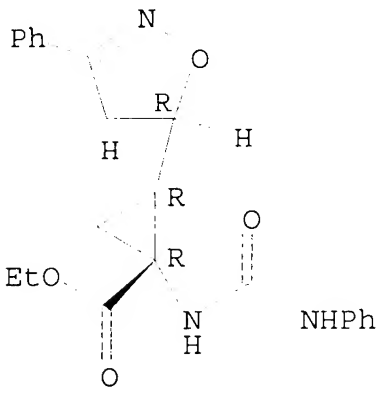
RN 213316-37-1 HCA
CN Cyclopropanecarboxylic acid, 2-[(5R)-4,5-dihydro-3-methyl-5-isoxazolyl]-1-[[(phenylamino)carbonyl]amino]-, ethyl ester, (1S,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



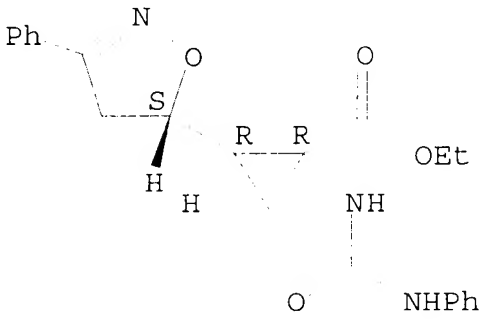
RN 213316-38-2 HCA
CN Cyclopropanecarboxylic acid, 2-[(5R)-4,5-dihydro-3-phenyl-5-isoxazolyl]-1-[[(phenylamino)carbonyl]amino]-, ethyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



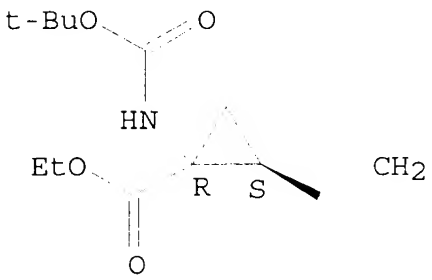
RN 213316-39-3 HCA
CN Cyclopropanecarboxylic acid, 2-[(5R)-4,5-dihydro-3-phenyl-5-isoxazolyl]-1-[[(phenylamino)carbonyl]amino]-, ethyl ester, (1S,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 213316-49-5 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-ethenyl-, ethyl ester, (1R,2S)-rel- (9CI) (CA INDEX NAME)

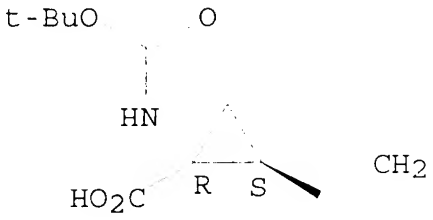
Relative stereochemistry.



RN 213316-50-8 HCA

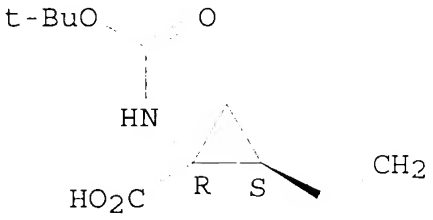
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-ethenyl-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



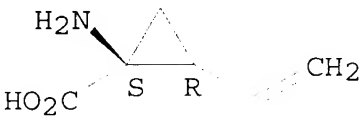
RN 213316-50-8 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-ethenyl-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



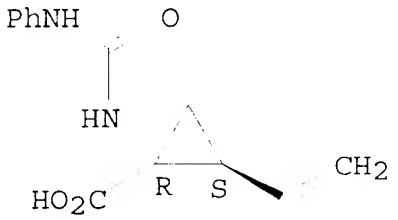
RN 213316-51-9 HCA
CN Cyclopropanecarboxylic acid, 1-amino-2-ethenyl-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



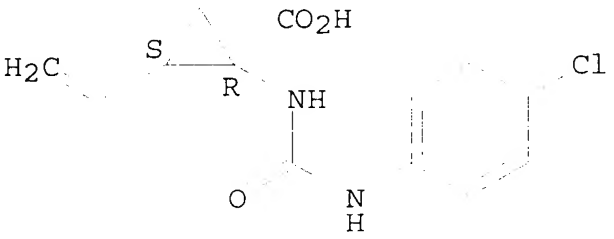
RN 213316-52-0 HCA
CN Cyclopropanecarboxylic acid, 2-ethenyl-1-[[(phenylamino)carbonyl]amino]-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



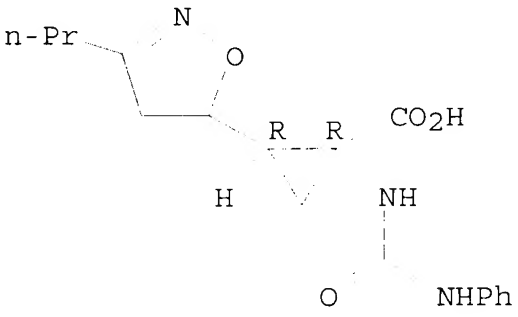
RN 213316-53-1 HCA
CN Cyclopropanecarboxylic acid, 1-[[[(4-chlorophenyl)amino]carbonyl]amino]-2-ethenyl-, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



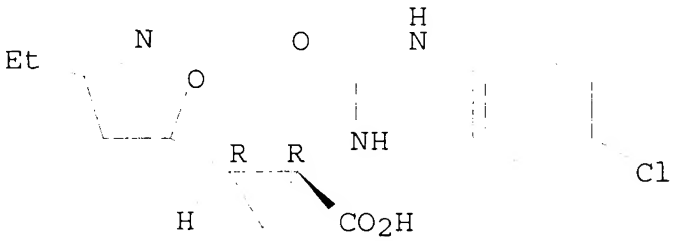
RN 213316-54-2 HCA
CN Cyclopropanecarboxylic acid, 2-(4,5-dihydro-3-propyl-5-isoxazolyl)-1-[[(phenylamino)carbonyl]amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



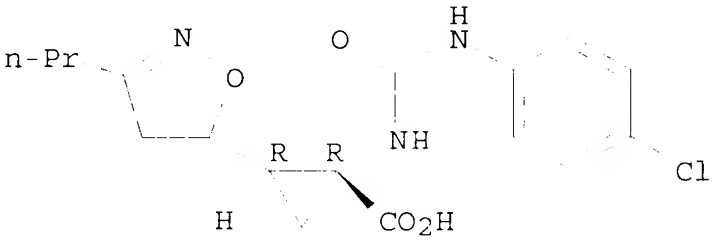
RN 213316-56-4 HCA
CN Cyclopropanecarboxylic acid, 1-[[[(4-chlorophenyl)amino]carbonyl]amino]-2-(3-ethyl-4,5-dihydro-5-isoxazolyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



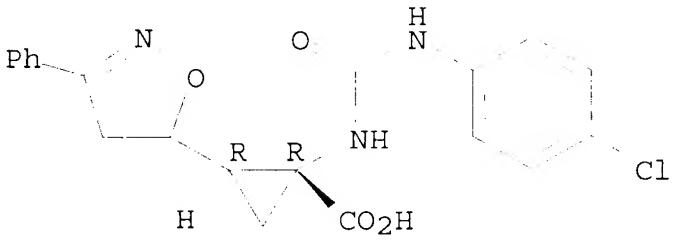
RN 213316-58-6 HCA
CN Cyclopropanecarboxylic acid, 1-[[[(4-chlorophenyl)amino]carbonyl]amino]-2-(4,5-dihydro-3-propyl-5-isoxazolyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



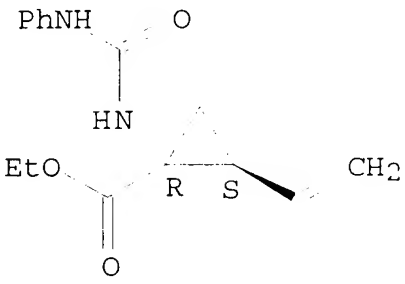
RN 213316-59-7 HCA
CN Cyclopropanecarboxylic acid, 1-[[[(4-chlorophenyl)amino]carbonyl]amino]-2-(4,5-dihydro-3-phenyl-5-isoxazolyl)-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **213316-33-7P**
(stereoselective solid-phase synthesis of novel hydantoin- and isoxazoline-contg. spiro compds.)
RN 213316-33-7 HCA
CN Cyclopropanecarboxylic acid, 2-ethenyl-1-[[(phenylamino)carbonyl]amino]-, ethyl ester, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 79-24-3, Nitroethane 103-71-9, Phenyl isocyanate, reactions
104-12-1, 4-Chlorophenyl isocyanate 622-42-4, .alpha.-Nitrotoluene
1195-45-5, 4-Fluorophenyl isocyanate 1476-11-5 25322-01-4,
Nitropropane 52006-62-9, Nitrobutane 199532-82-6
213316-20-2
(stereoselective solid-phase synthesis of novel hydantoin- and isoxazoline-contg. spiro compds.)
IT **27314-05-2DP**, polymer-bound **199532-88-2P**
207729-00-8P 210709-45-8DP, polymer-bound
213316-20-2DP, polymer-bound **213316-21-3DP**,
polymer-bound **213316-22-4DP**, polymer-bound
213316-23-5DP, polymer-bound **213316-24-6DP**,
polymer-bound **213316-25-7DP**, polymer-bound
213316-26-8DP, polymer-bound **213316-27-9DP**,
polymer-bound **213316-28-0DP**, polymer-bound
213316-32-6P 213316-34-8P 213316-35-9P
213316-36-0P 213316-37-1P 213316-38-2P
213316-39-3P 213316-49-5P 213316-50-8DP,
polymer-bound **213316-50-8P 213316-51-9DP**,
polymer-bound **213316-52-0DP**, polymer-bound
213316-53-1DP, polymer-bound **213316-54-2DP**,
polymer-bound **213316-56-4DP**, polymer-bound
213316-58-6DP, polymer-bound **213316-59-7DP**,
polymer-bound
(stereoselective solid-phase synthesis of novel hydantoin- and isoxazoline-contg. spiro compds.)
IT 199532-86-0P 199532-99-5P 199533-00-1P 213316-29-1P
213316-30-4P 213316-31-5P **213316-33-7P** 213316-40-6P
213316-42-8P 213316-43-9P 213316-44-0P 213316-45-1P
213316-46-2P 213316-47-3P 213316-48-4P
(stereoselective solid-phase synthesis of novel hydantoin- and isoxazoline-contg. spiro compds.)

L27 ANSWER 8 OF 16 HCA COPYRIGHT 2003 ACS
125:196380 Preparation of a library of compounds by solid-phase synthesis.. Kobylecki, Ryszard Jurek; Gardner, John Mark Francis (Pfizer Limited, UK). Brit. UK Pat. Appl. GB 2295152 A1 19960522,

37 pp. (English). CODEN: BAXXDU. APPLICATION: GB 1994-23332 19941118.

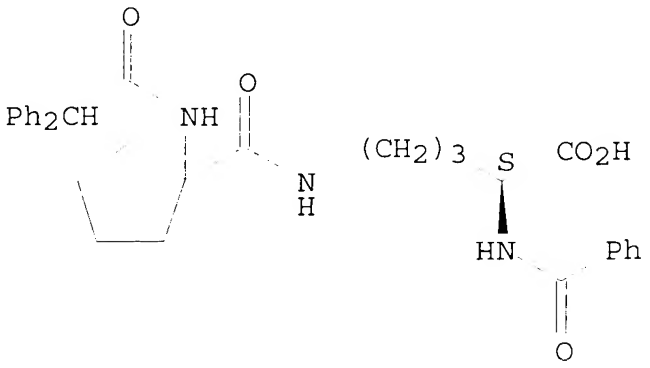
AB A method of making a library of compds. comprises the following steps: (a) individually identifying a plurality of discrete reaction zones defined on laminar solid support material; (b) charging each of said reaction zones with a starting material; (c) sub-dividing the reaction zones into .gtoreq.2 initial batches; (d) applying .gtoreq.2 different reagents, 1 to each of the reaction zones in each initial batch, and recording the identity of those reaction zones to which each of said different reagents is applied; (e) subjecting all reaction zones to reaction conditions which promote reaction to completion; (f) further sub-dividing the reaction zones into .gtoreq.2 alternative batches; (g) applying .gtoreq.2 different reagents, one to each of the reaction zones in each alternative batch, and recording the identity of those reaction zones to which each of said different reagents is applied; (h) subjecting all reaction zones to reaction conditions which promote reaction to completion, and (i) repeating steps (f) to (h) as desired. The solid support may be amine-derivatized cellulose sheets, or laminated materials such as a functionalized resin (aminomethylpolystyrene) sandwiched (with a polyethylene) between porous inert sheets (non-woven fibrous polypropylene). Thus, a 1677 component peptoid library was prepd. on aminopropyl-functionalized paper divided into 43 columns and 39 rows. The 43 columns were divided and sep. functionalized with activated FMOC-protected amino acid derivs. followed by deprotection and acetylation of residual amine functionality; the strips were stacked and cut into sets of reaction zones, each set was coupled with a second amino acid deriv. followed by deprotection. Finally, the combined set of 1677 reaction zones was treated with diphenylacetyl chloride and Hunig's base followed by individual cleavage of the trimeric products from their reaction zones.

IT **180511-22-2P**
(prepn. of a library of compds. by solid-phase synthesis)

RN 180511-22-2 HCA

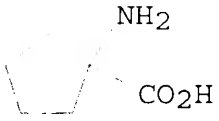
CN L-Ornithine, N2-benzoyl-N5-[[1-[(diphenylacetyl)amino]cyclopentyl]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07K001-04
ICS B32B005-26; B32B007-12; D21H017-26
CC 34-3 (Amino Acids, Peptides, and Proteins)
IT Combinatorial library
Merrifield synthesis
(prepn. of a library of compds. by solid-phase synthesis)
IT 15373-56-5P 23828-14-0P 34027-62-8P 35193-18-1P 51352-46-6P
54925-87-0P 58725-29-4P 71227-74-2P 71730-64-8P 72578-95-1P
72829-55-1P 81161-89-9P 85807-00-7P 88992-14-7P 91290-35-6P
97812-04-9P 114019-68-0P 133706-67-9P 158052-68-7P
180511-20-0P **180511-22-2P** 180511-23-3P 180511-24-4P
180511-26-6P 180511-27-7P 180511-29-9P 180511-31-3P
180511-32-4P 180511-34-6P 180511-36-8P 180511-37-9P
180511-38-0P 180511-39-1P 180511-40-4P 180511-41-5P
(prepn. of a library of compds. by solid-phase synthesis)

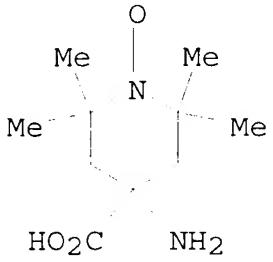
L27 ANSWER 9 OF 16 HCA COPYRIGHT 2003 ACS
124:261653 Solid phase synthesis of hydantoins using a carbamate linker and a novel cyclization/cleavage step. Dressman, Bruce A.; Spangle, Larry A.; Kaldor, Stephen W. (Lilliy Res. Lab., Lilly Corporate Center, Indianapolis, IN, 46285, USA). Tetrahedron Letters, 37(7), 937-40 (English) 1996. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier.
AB An 800 compd. hydantoin library has been constructed using a diverse set of 20 amino acids and over 80 primary amines. Amino acids were attached via their N-termini to (hydroxymethyl)polystyrene using a carbamate linker. Bound amino acids were converted to their corresponding amides and then cyclized under basic conditions to give hydantoins in high purities.
IT **52-52-8**, 1-Aminocyclopentanecarboxylic acid
(solid phase synthesis of hydantoins using a carbamate linker and a novel cyclization/cleavage step)
RN 52-52-8 HCA
CN Cyclopentanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 28
ST **Merrifield** synthesis hydantoin combinatorial library; amino acid primary amine cyclocondensation
IT Combinatorial library
Merrifield synthesis
(solid phase synthesis of hydantoins using a carbamate linker and a novel cyclization/cleavage step)
IT **52-52-8**, 1-Aminocyclopentanecarboxylic acid 63-91-2, Phenylalanine, reactions 71-00-1, Histidine, reactions 73-22-3, Tryptophan, reactions 100-46-9, Benzylamine, reactions 103-01-5, N-Phenylglycine 502-32-9, Leucinol 3060-50-2, 2,2-Diphenylglycine 3731-53-1, 4-Aminomethylpyridine 3963-62-0, 2,2-Diphenylethylamine 5805-57-2, 2-Aminomethylbenzimidazole 7568-93-6, 2-Amino-1-phenylethanol 7693-46-1, p-Nitrophenyl chloroformate 13211-31-9, Valine tert-butyl ester 18822-59-8, O-tert-Butyltyrosine 27431-62-5, N,N-Diethyl-1,4-butanediamine 35186-99-3, 1,2,3,4-Tetrahydroisoquinoline-3-carboxylic acid 68076-36-8, N-tert-Butoxycarbonyl-1,4-butanediamine
(solid phase synthesis of hydantoins using a carbamate linker and a novel cyclization/cleavage step)

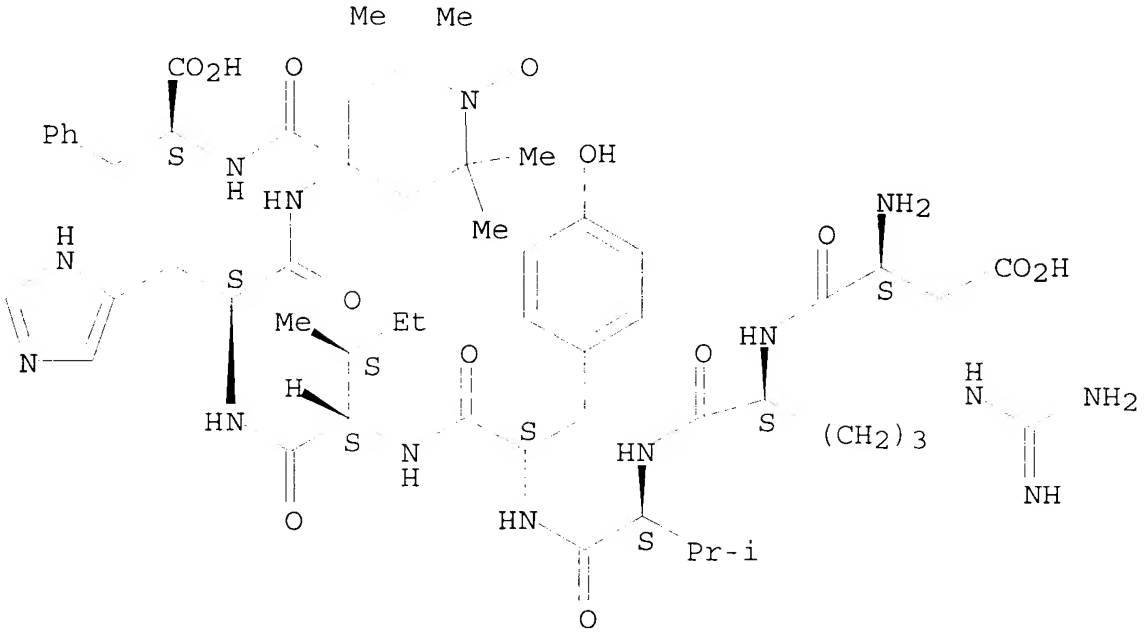
L27 ANSWER 10 OF 16 HCA COPYRIGHT 2003 ACS
120:31213 A novel spin-labeled amino acid derivative for use in peptide synthesis: (9-fluorenylmethyloxycarbonyl)-2,2,6,6-tetramethylpiperidine-N-oxyl-4-amino-4-carboxylic acid. Marchetto, Reinaldo; Schreier, Shirley; Nakaie, Clovis R. (Dep. Biophys., Es. Paulista Med., Sao Paulo, 04044-020, Brazil). Journal of the American Chemical Society, 115(23), 11042-3 (English) 1993. CODEN: JACSAT. ISSN: 0002-7863.
AB A method for the solid phase synthesis of peptides contg. a spin-labeled amino acid at a non-terminal position of the peptide chain is described, using the N.alpha.-Fmoc (9-fluorenylmethyloxycarbonyl) deriv. of the spin labeled amino acid 2,2,6,6-tetramethylpiperidine-N-oxyl-4-amino-4-carboxylic acid (TOAC). An analog of the octapeptide hormone angiotensin II in which the Pro7 residue was replaced by TOAC (TOAC7-angiotensin II) was synthesized. The availability, for the first time, of a peptide analog contg. a spin labeled amino acid at an internal position may be valuable for studies of peptides conformation and their interactions with macromols. and membranes of biol. interest.
IT **15871-57-5**
(fluorenylmethoxycarbonylation of)
RN 15871-57-5 HCA
CN 1-Piperidinyloxy, 4-amino-4-carboxy-2,2,6,6-tetramethyl- (9CI) (CA

INDEX NAME)

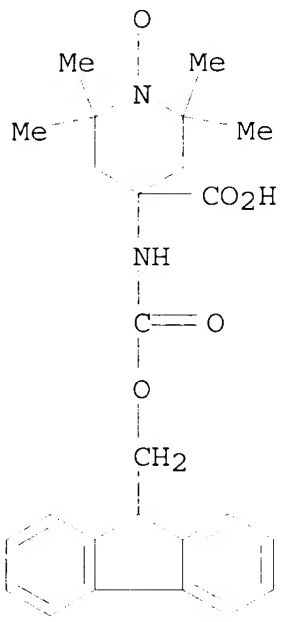


IT **151842-58-9P**
(prepn. and ESR of)
RN 151842-58-9 HCA
CN Angiotensin II, 5-L-isoleucine-7-(4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarboxylic acid)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

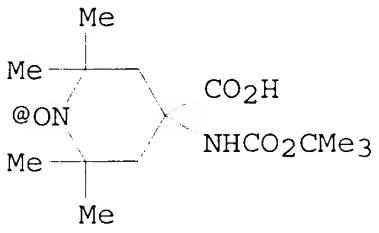


IT **93372-25-9P**
(prepn. and solid-phase peptide coupling reaction of)
RN 93372-25-9 HCA
CN 1-Piperidinyloxy, 4-carboxy-4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



CC 34-3 (Amino Acids, Peptides, and Proteins)
IT **15871-57-5**
(fluorenylmethoxycarbonylation of)
IT **151842-58-9P**
(prepn. and ESR of)
IT **93372-25-9P**
(prepn. and solid-phase peptide coupling reaction of)
IT 35661-40-6D, **Wang** resin-bound
(solid-phase peptide synthesis with)

L27 ANSWER 11 OF 16 HCA COPYRIGHT 2003 ACS
112:56666 Synthetic and physicochemical studies of benzhydrylamine resins with different substitution levels: implications for solid phase peptide synthesis. Nakaie, Clovis R.; Marchetto, Reinaldo; Schreier, Shirley; Paiva, Antonio C. M. (Dep. Biophys., Esc. Paulista Med., Sao Paulo, 04034, Brazil). Pept.: Chem. Biol., Proc. Am. Pept. Symp. 10th, Meeting Date 1987, 249-51. Editor(s): Marshall, Garland R. ESCOM Sci. Pub.: Leiden, Neth. (English) 1988. CODEN: 56MDA6.
GI



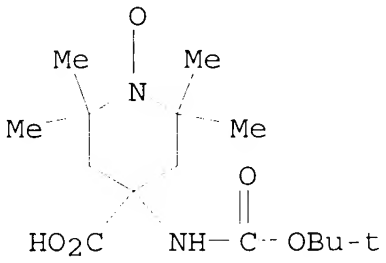
I

AB A symposium on the swelling properties of benzhydrylamine resins with substitutions ranging from 0.05 to 2.2 mmol/g. The swelling and pendant peptide mobility was measured using nitroxyl amino acid I and ESR.

IT **124843-12-5D**, amide with benzhydrylamine resin
(mobility of, by ESR line broadening)

RN 124843-12-5 HCA

CN 1-Piperidinyloxy, 4-carboxy-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22

ST benzyhydrylamine resin swelling properties symposium; nitroxyl amino acid ESR mobility symposium; **Merrifield** synthesis benzhydrylamine resin symposium

IT **Merrifield** synthesis
(benzhydrylamine resin for, swelling properties and pendant group mobilities of)

IT **124843-12-5D**, amide with benzhydrylamine resin
(mobility of, by ESR line broadening)

L27 ANSWER 12 OF 16 HCA COPYRIGHT 2003 ACS

111:233555 Amino acids and peptides. Part CCVII. Synthesis and properties of analogs of vasopressin with 1-aminocyclopropane-1-carboxylic acid in position 9. Prochazka, Zdenko; Ancans, Juris E.; Slaninova, Jirina; Machova, Alena; Barth, Tomislav; Skopkova, Jana; Budesinsky, Milos; Pavlikova, Frantiska; Lebl, Michal (Inst. Org. Chem. Biochem., Slovak Acad. Sci., Prague, 16610/6, Czech.). Collection of Czechoslovak Chemical Communications, 53(11A), 2604-16 (English) 1988. CODEN: CCCCAK. ISSN: 0010-0765. OTHER SOURCES: CASREACT 111:233555.

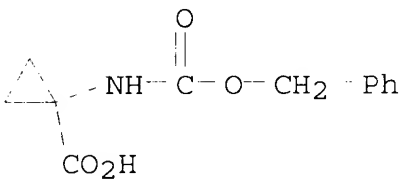
GI For diagram(s), see printed CA Issue.

AB Title vasopressin analogs I (Acc = 1-aminocyclopropane-1-carboxylic acid; R = H, X = Lys, Arg; R = H-Gly-Gly-Gly, X = Lys) were prepd. by the solid-phase method on benzhylamine resin. The dubious value of the biol. activity of [Lys8,D-Ala9]vasopressin was reevaluated and [Lys8,L-Ala9]vasopressin was also synthesized and tested for the comparison. Differences in soln. conformation of these two analogs were studied by 1H and 13C NMR spectroscopy. Biol. activities of all analogs were either significantly lowered or almost completely eliminated.

IT **84677-06-5**
(amidation of, with benzylhydrylamine resin)

RN 84677-06-5 HCA

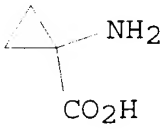
CN Cyclopropanecarboxylic acid, 1-[[(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



IT **22059-21-8DP**, 1-Aminocyclopropane-1-carboxylic acid, vasopressin analogs contg. **123860-74-2P** **123860-75-3P** **123860-84-4P** **123860-85-5P** **123886-57-7P** **123886-58-8P**
(prepn. and biol. activity of)

RN 22059-21-8 HCA

CN Cyclopropanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

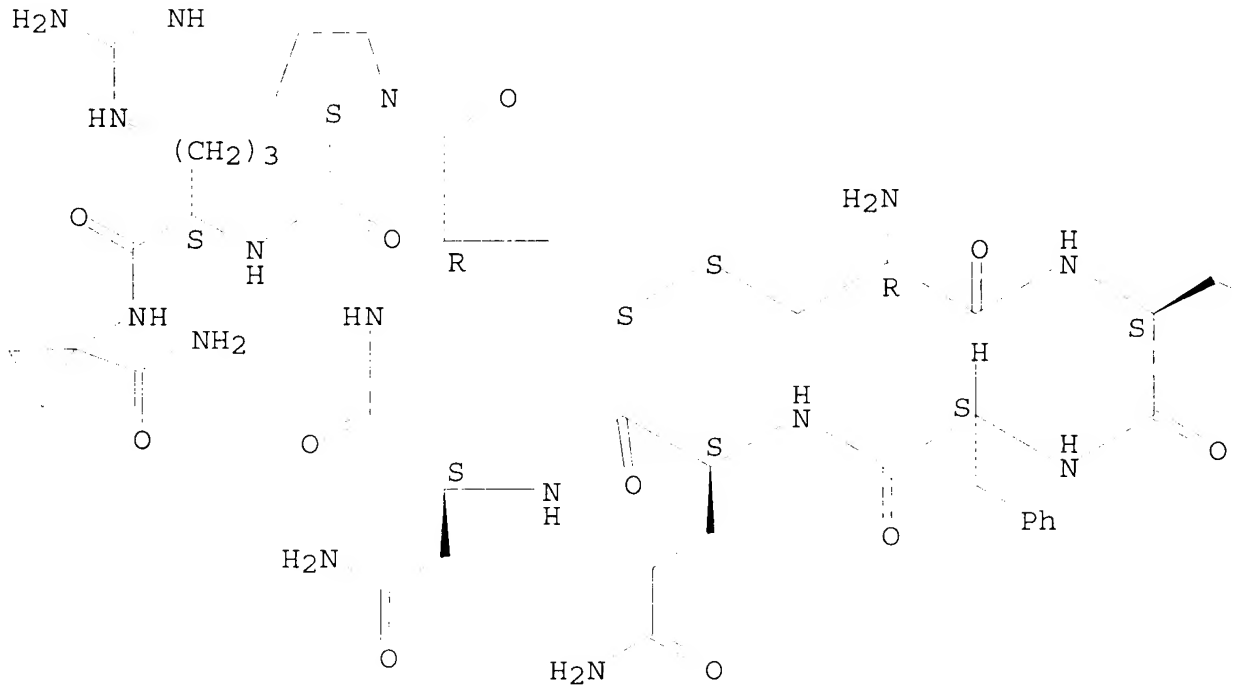


RN 123860-74-2 HCA

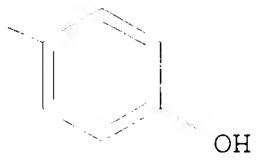
CN Vasopressin, 8-L-arginine-9-(1-aminocyclopropanecarboxamide)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



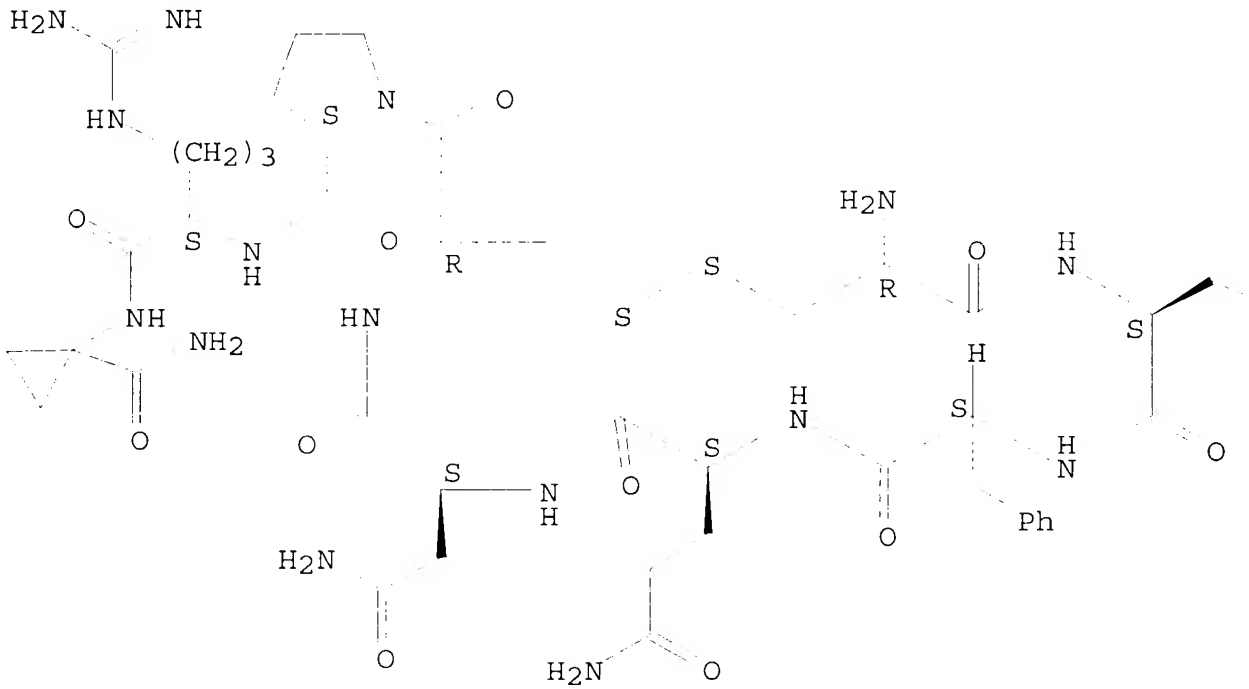
RN 123860-75-3 HCA
CN Vasopressin, 8-L-arginine-9-(1-aminocyclopropanecarboxamide)-, tris(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 123860-74-2
CMF C48 H67 N15 O12 S2

Absolute stereochemistry.

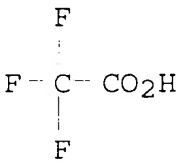
PAGE 1-A



PAGE 1-B

CM 2

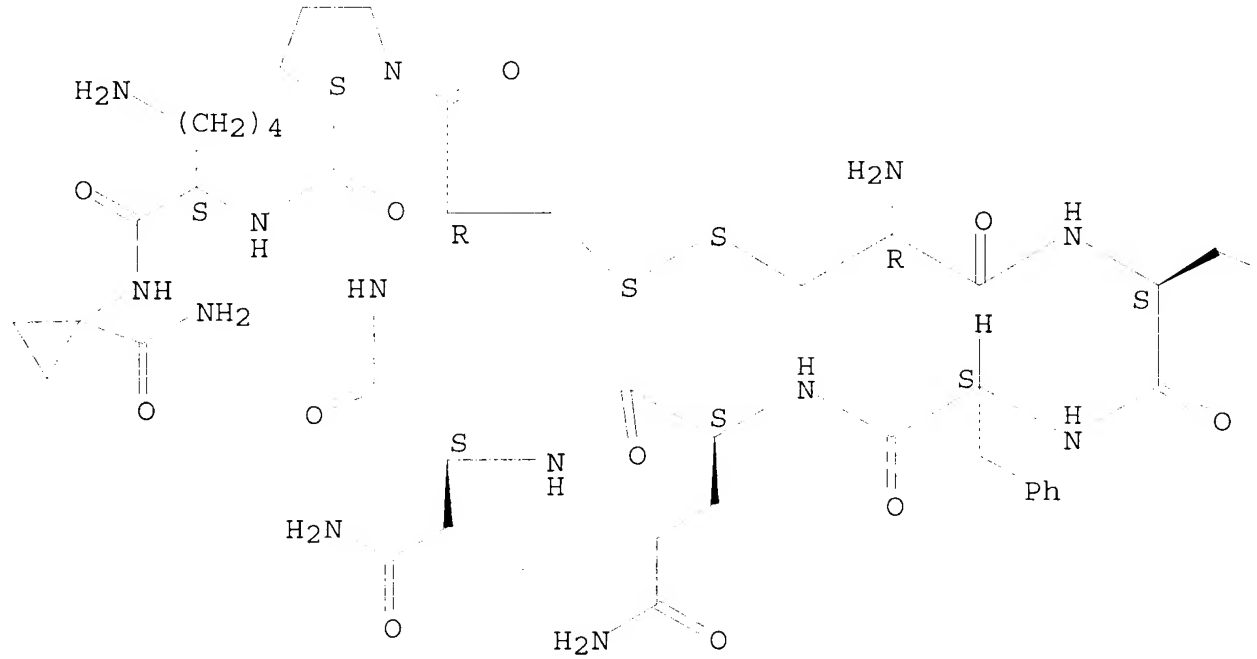
CRN 76-05-1
CMF C2 H F3 O2



RN 123860-84-4 HCA
CN Vasopressin, 8-L-lysine-9-(1-aminocyclopropanecarboxamide)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

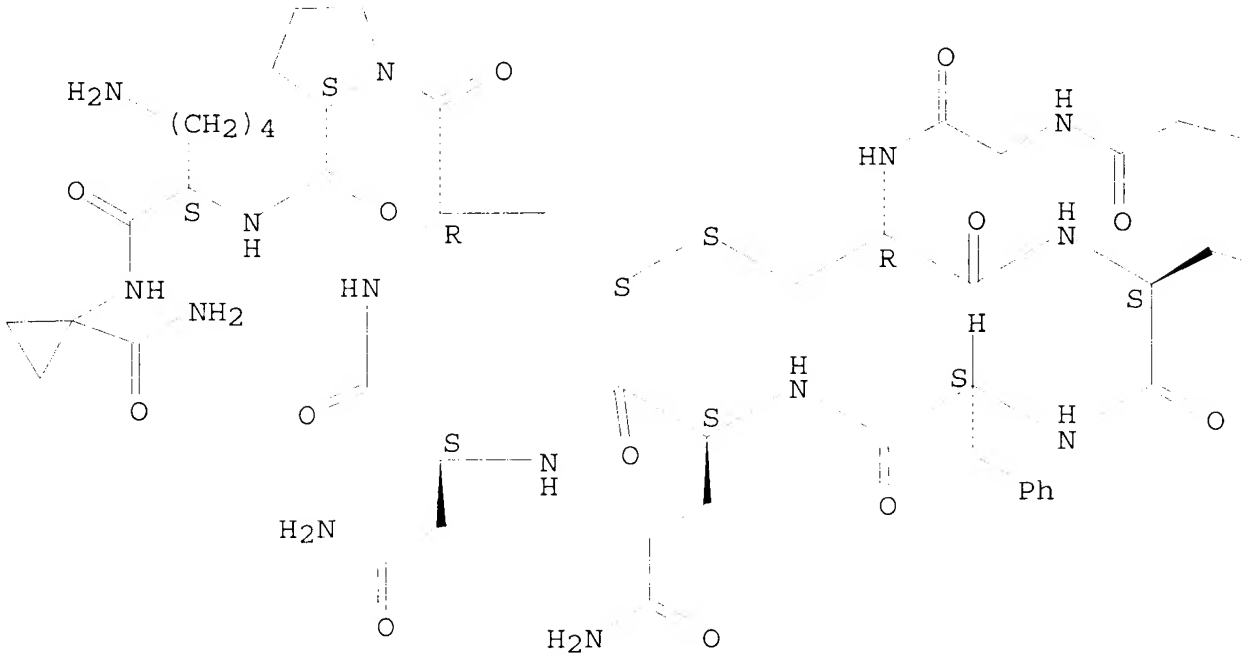


PAGE 1-B

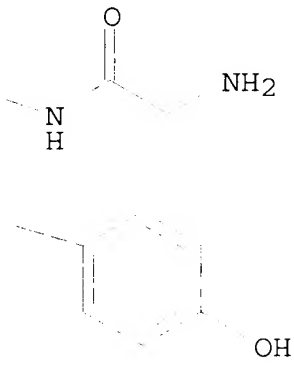
RN 123860-85-5 HCA
CN L-Lysinamide, glycylglycylglycyl-L-cysteinyl-L-tyrosyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-L-cysteinyl-L-prolyl-N-[1-(aminocarbonyl)cyclopropyl]-, cyclic (4.fwdarw.9)-disulfide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



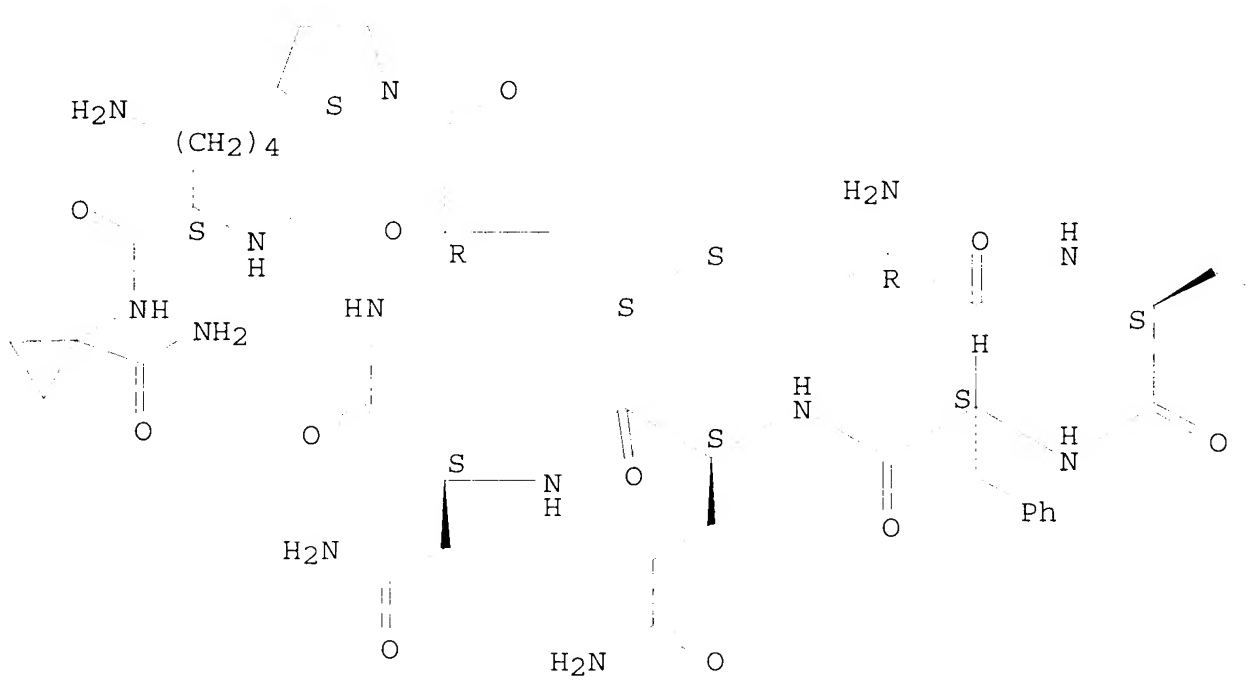
RN 123886-57-7 HCA
CN Vasopressin, 8-L-lysine-9-(1-aminocyclopropanecarboxamide)-, tetraacetate (salt) bis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

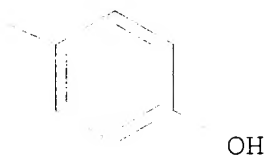
CRN 123860-84-4
CMF C48 H67 N13 O12 S2

Absolute stereochemistry.

PAGE 1-A

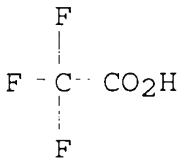


PAGE 1-B



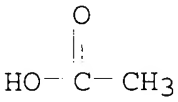
CM 2

CRN 76-05-1
CMF C2 H F3 O2



CM 3

CRN 64-19-7
CMF C2 H4 O2



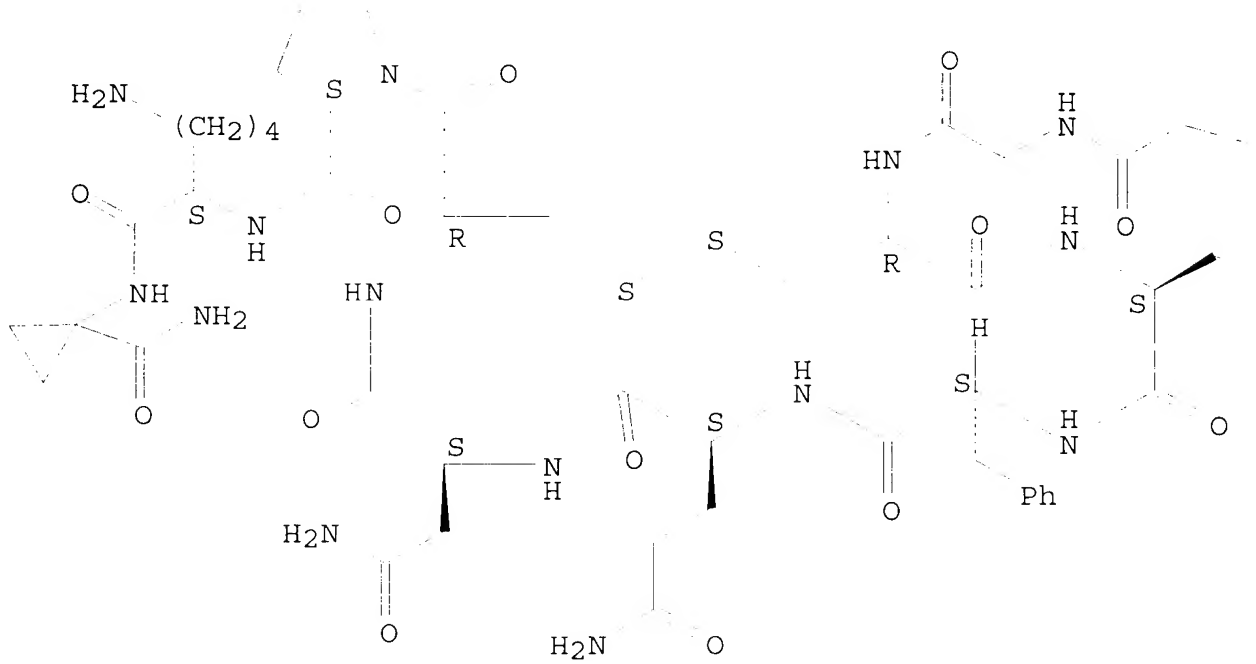
RN 123886-58-8 HCA
CN L-Lysinamide, glycylglycylglycyl-L-cysteinyl-L-tyrosyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-L-cysteinyl-L-prolyl-N-[1-(aminocarbonyl)cyclopropyl]-, cyclic (4.fwdarw.9)-disulfide, pentakis(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

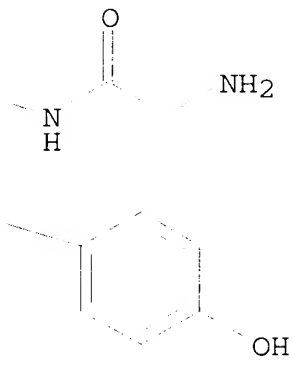
CRN 123860-85-5
CMF C54 H76 N16 O15 S2

Absolute stereochemistry.

PAGE 1-A

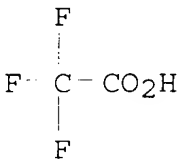


PAGE 1-B



CM 2

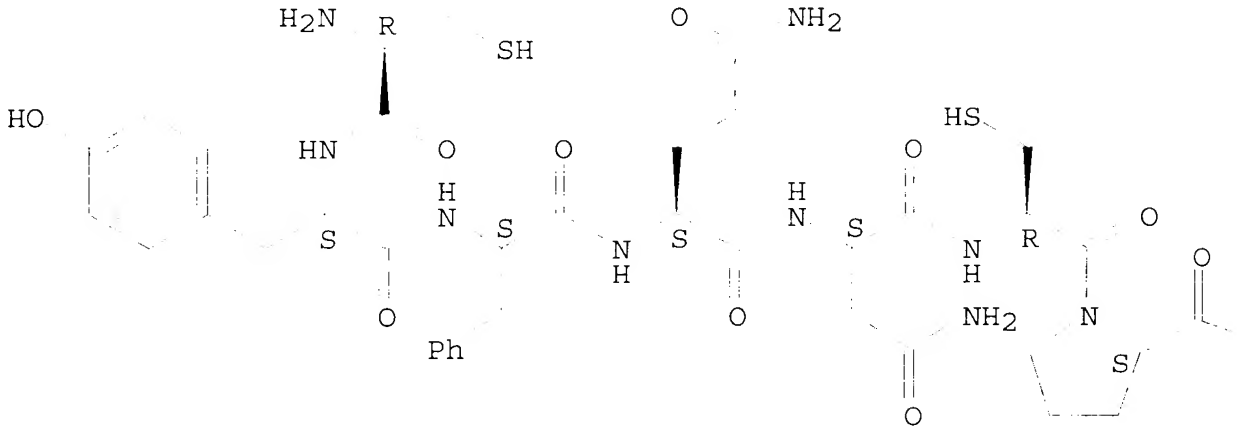
CRN 76-05-1
CMF C2 H F3 O2



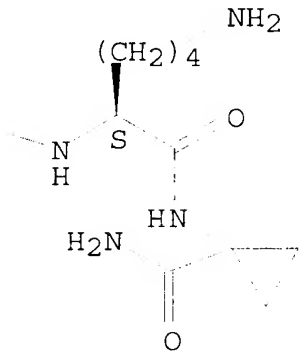
IT **123860-78-6P 123860-79-7P 123860-81-1P**
(prepn. and oxidative cyclization of)
RN 123860-78-6 HCA
CN L-Lysinamide, L-cysteinyl-L-tyrosyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-L-cysteinyl-L-prolyl-N-[1-(aminocarbonyl)cyclopropyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



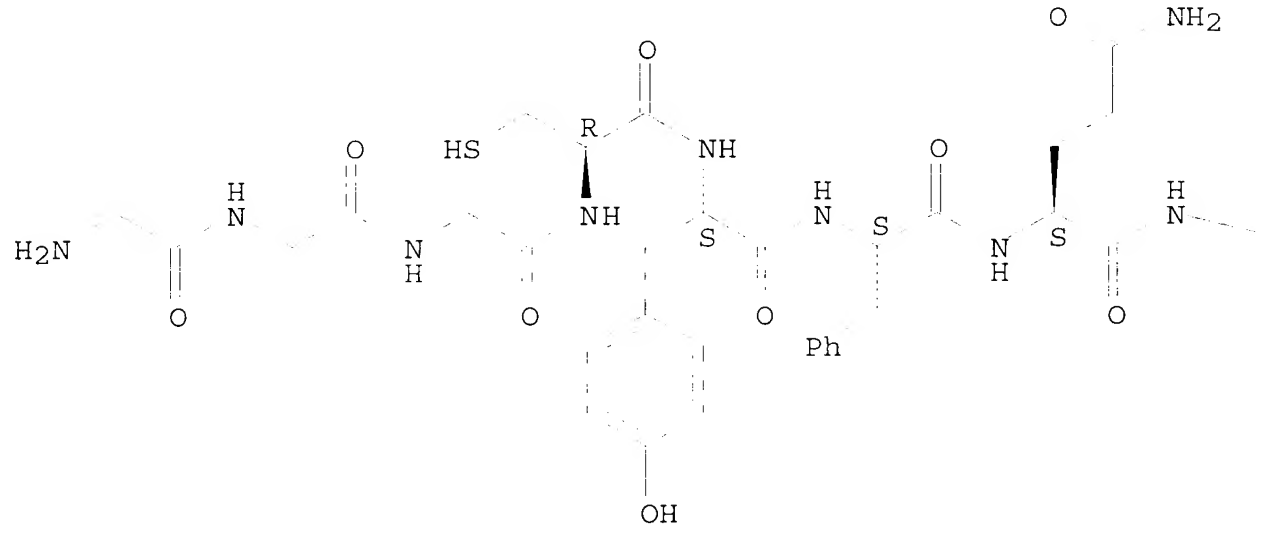
PAGE 1-B



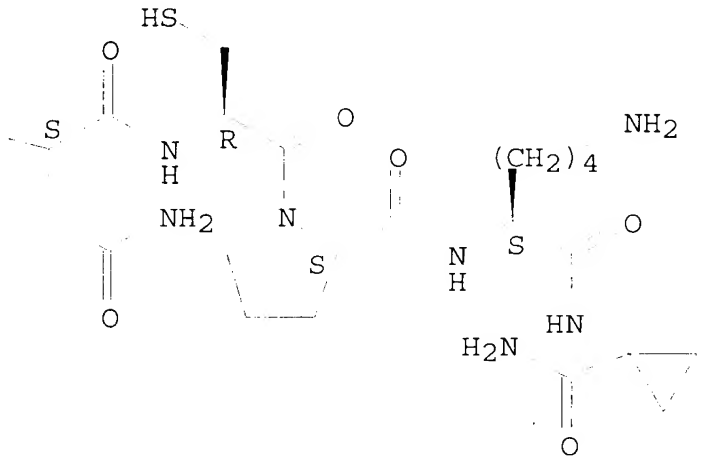
RN 123860-79-7 HCA
CN L-Lysinamide, glycylglycylglycyl-L-cysteinyl-L-tyrosyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-L-cysteinyl-L-prolyl-N-[1-(aminocarbonyl)cyclopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



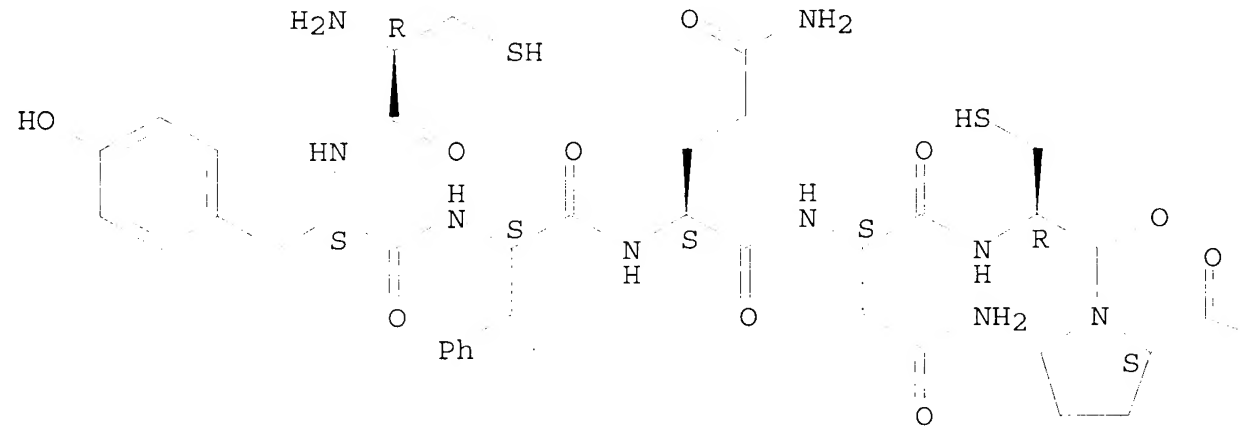
PAGE 1-B



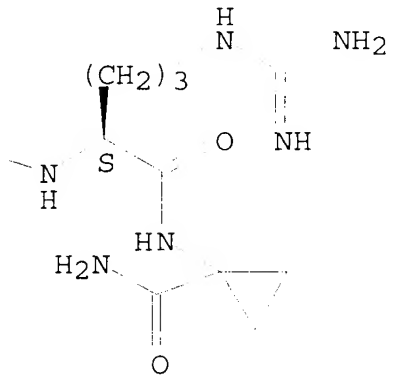
RN 123860-81-1 HCA
CN L-Argininamide, L-cysteinyl-L-tyrosyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-L-cysteinyl-L-prolyl-N-[1-(aminocarbonyl)cyclopropyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



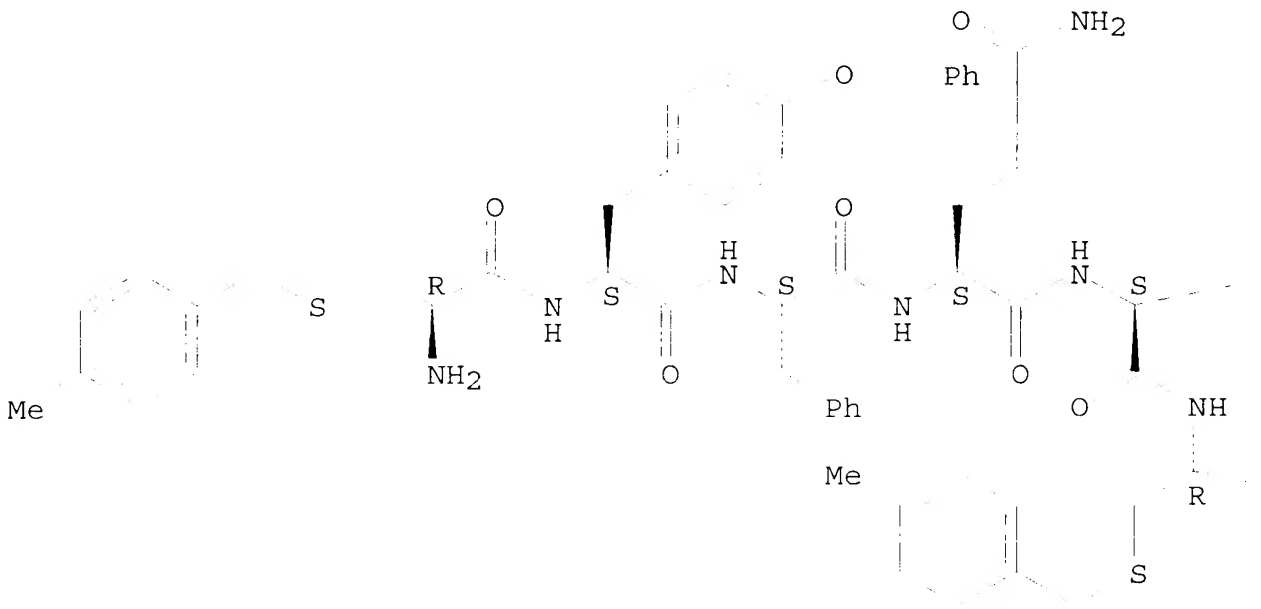
IT **123860-77-5DP**, amide with benzhydrylamine resin
123860-80-0DP, amide with benzhydrylamine resin
(prepn. and resin cleavage-deblocking of)

RN 123860-77-5 HCA

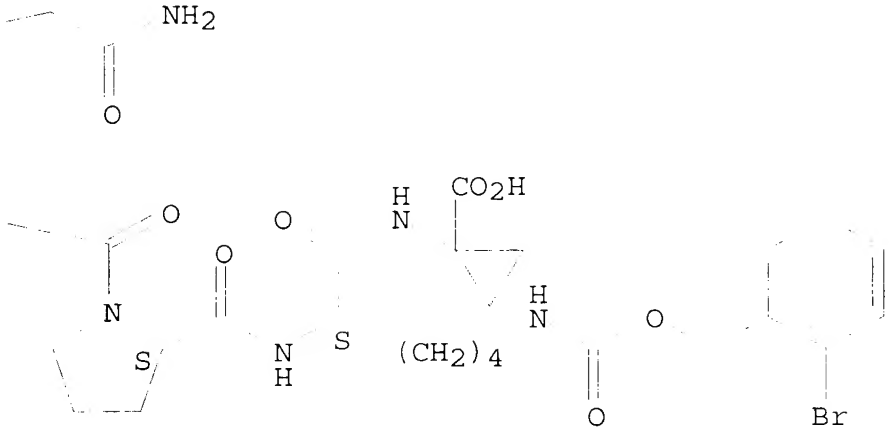
CN L-Lysinamide, S-[(4-methylphenyl)methyl]-L-cysteinyl-O-(phenylmethyl)-L-tyrosyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-S-[(4-methylphenyl)methyl]-L-cysteinyl-L-prolyl-N6-[[(2-bromophenyl)methoxy]carbonyl]-N-(1-carboxycyclopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



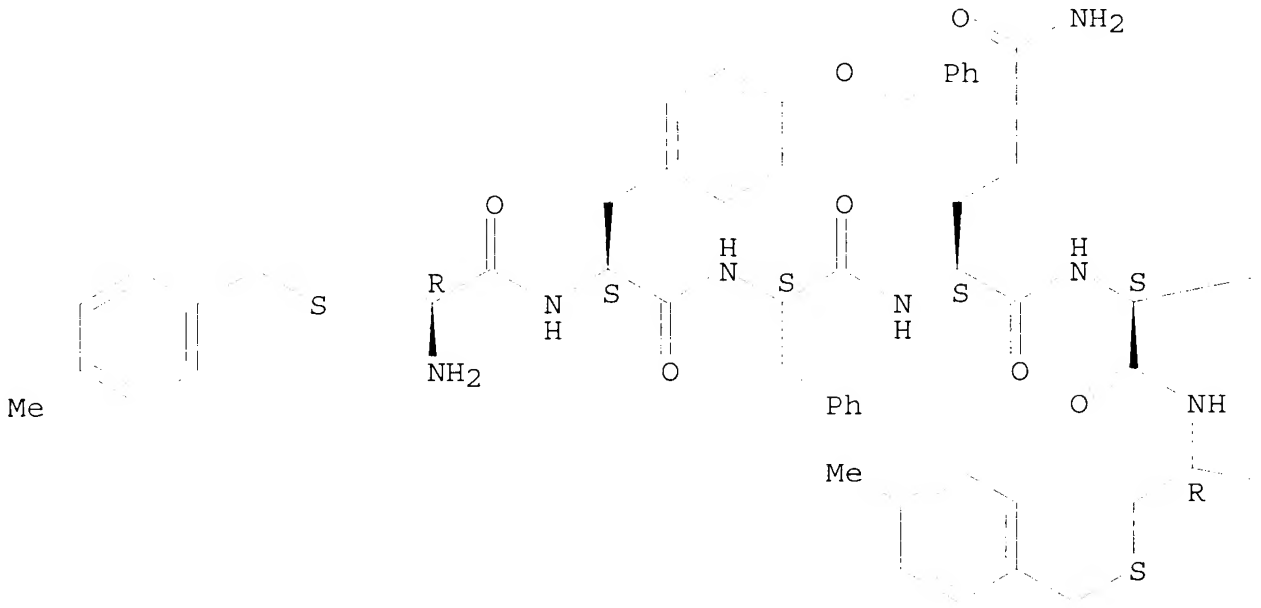
PAGE 1-B



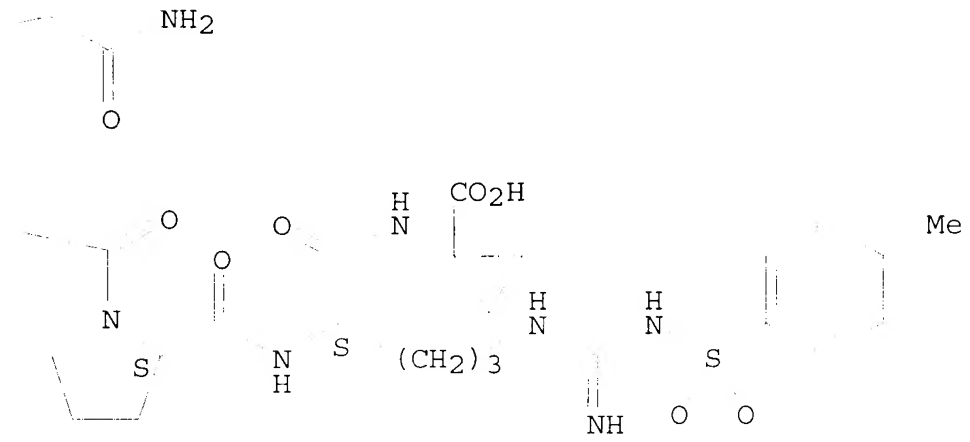
RN 123860-80-0 HCA
CN L-Ornithinamide, S-[(4-methylphenyl)methyl]-L-cysteinyl-O-(phenylmethyl)-L-tyrosyl-L-phenylalanyl-L-glutaminyl-L-asparaginyl-S-[(4-methylphenyl)methyl]-L-cysteinyl-L-prolyl-N-(1-carboxycyclopropyl)-N5-[imino[[(4-methylphenyl)sulfonyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

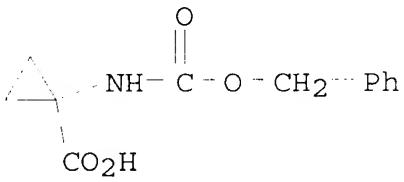
PAGE 1-A



PAGE 1-B



IT **84677-06-5DP**, amide with benzhydrylamine resin
(prepn. and solid-phase peptide synthesis with)
RN 84677-06-5 HCA
CN Cyclopropanecarboxylic acid, 1-[[(phenylmethoxy)carbonyl]amino]-
(9CI) (CA INDEX NAME)



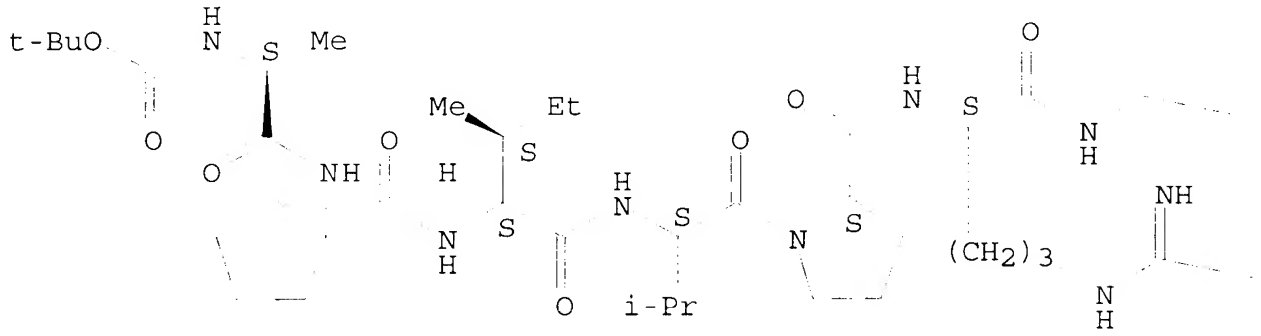
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 2
ST aminocyclopropanecarboxylic vasopressin analog **Merrifield** synthesis; structure activity aminocyclopropanecarboxylic vasopressin analog
IT **84677-06-5**
(amidation of, with benzylhydrylamine resin)
IT 11000-17-2DP, Vasopressin, aminocyclopropanecarboxylic acid-contg. analogs 14316-02-0P **22059-21-8DP**, 1-Aminocyclopropane-1-carboxylic acid, vasopressin analogs contg. **123860-74-2P** **123860-75-3P** **123860-84-4P** **123860-85-5P**

123886-57-7P 123886-58-8P
(prepn. and biol. activity of)
IT **123860-78-6P 123860-79-7P 123860-81-1P**
123860-83-3P
(prepn. and oxidative cyclization of)
IT **123860-77-5DP**, amide with benzhydrylamine resin
123860-80-0DP, amide with benzhydrylamine resin
123860-82-2DP, amide with benzhydrylamine resin
(prepn. and resin cleavage-deblocking of)
IT **84677-06-5DP**, amide with benzhydrylamine resin
(prepn. and solid-phase peptide synthesis with)

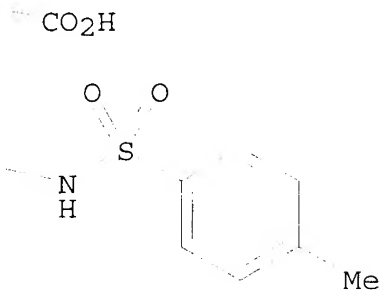
L27 ANSWER 13 OF 16 HCA COPYRIGHT 2003 ACS
97:39360 Enhancement of peptide coupling reactions by 4-dimethylaminopyridine. Wang, S. S.; Wang, B. S. H.; Tam, J. P.; Merrifield, R. B. (Peninsula Lab., Inc., Belmont, CA, 94002, USA). Pept.: Synth., Struct., Funct., Proc. Am. Pept. Symp., 7th, 197-9. Editor(s): Rich, Daniel H.; Gross, Erhard. Pierce Chem. Co.: Rockford, Ill. (English) 1981. CODEN: 47LMAO.
AB 4-Dimethylaminopyridine (DMAP) enhanced DCC-mediated peptide couplings in the solid-phase synthesis of Boc-Ala-Cle-Ile-Val-Pro-Arg(Tos)-Gly-OCH2-resin (Boc = Me3CO2C, Tos = tosyl, Cle = cycloleucine residue); the DCC/DMAP procedure gave near quant. couplings in the sterically hindered region of Cle-Ile-Val. The racemization during the coupling of Boc-Ile-OH with H-Val-OCH2-resin by DCC/DMAP was similar to that for the DCC method, whereas significant racemization occurred during the coupling of Boc-Phe-OH with H-Glu(OCH2Ph)-OCH2-resin via the DCC/DMAP method. Racemization during sym. anhydride coupling for the same synthesis was reduced by the addn. of DMAP.
IT **81136-53-0DP**, resin-bound
(prepn. of, by dicyclohexylcarbodiimide-dimethylaminopyridine-mediated peptide coupling reactions)
RN 81136-53-0 HCA
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-1-aminocyclopentanecarbonyl-L-isoleucyl-L-valyl-L-prolyl-N5-[imino[[(4-methylphenyl)sulfonyl]amino]methyl]-L-ornithyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



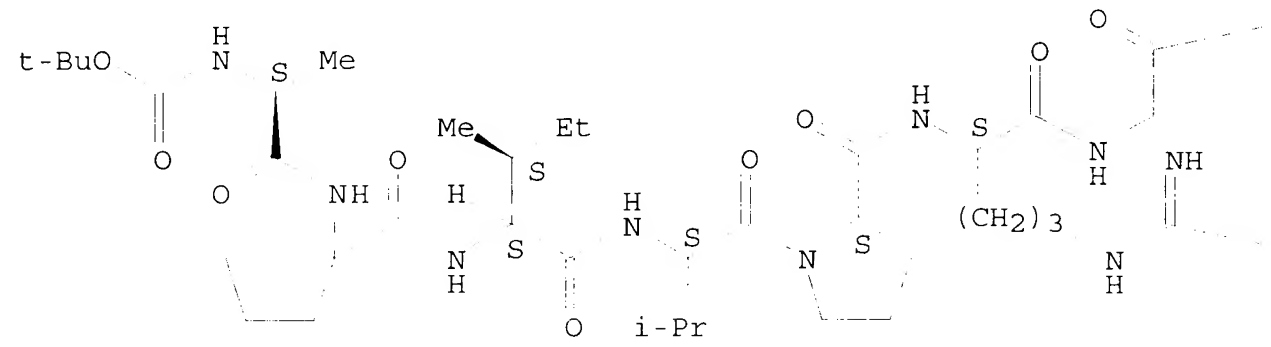
IT **81136-54-1P**
(prepn. of, by solid-phase method using dicyclohexylcarbodiimide-dimethylaminopyridine-mediated peptide coupling reaction)

RN 81136-54-1 HCA

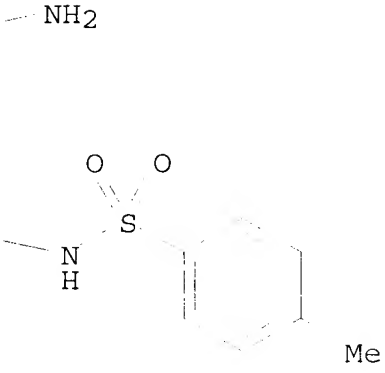
CN Glycinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-1-aminocyclopentanecarbonyl-L-isoleucyl-L-valyl-L-prolyl-N5-[imino[[(4-methylphenyl)sulfonyl]amino]methyl]-L-ornithyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 34-3 (Amino Acids, Peptides, and Proteins)
ST methylaminopyridine enhancement dicyclohexylcarbodiimide peptide coupling; carbodiimide peptide coupling dimethylaminopyridine enhancement; pyridine dimethylamino enhancement peptide coupling; sym anhydride peptide dimethylaminopyridine enhancement; **Merrifield** synthesis peptide dimethylaminopyridine enhancement; steric hindrance peptide coupling dimethylaminopyridine; racemization peptide coupling dimethylaminopyridine
IT **Merrifield** synthesis
(of peptides, dicyclohexylcarbodiimide-dimethylaminopyridine-mediated coupling reactions in)
IT **81136-53-0DP**, resin-bound
(prepn. of, by dicyclohexylcarbodiimide-dimethylaminopyridine-mediated peptide coupling reactions)
IT **81136-54-1P**
(prepn. of, by solid-phase method using dicyclohexylcarbodiimide-dimethylaminopyridine-mediated peptide coupling reaction)

L27 ANSWER 14 OF 16 HCA COPYRIGHT 2003 ACS
97:21108 Structural and conformational properties of peptides

interacting with the glutathione receptor of hydra. Cobb, Melanie H.; Heagy, Wyrta; Danner, Jean; Lenhoff, Howard M.; Marshall, Garland R. (Sch. Med., Washington Univ., St. Louis, MO, 63110, USA). Molecular Pharmacology, 21(3), 629-36 (English) 1982. CODEN: MOPMA3. ISSN: 0026-895X.

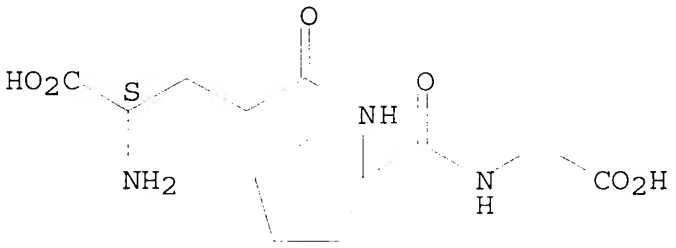
AB Structure-activity relations of the glutathione-induced feeding response in the freshwater coelenterate, Hydra attenuata, were studied to map structural and conformational properties of feeding response agonists. The .gamma.-glutamyl residue of glutathione contains essential binding sites for receptor interaction, without which antagonistic as well as agonistic properties are lost. Any structural alteration which perturbs either the .alpha.-amino or the .alpha.-carboxyl group or their relative spatial orientations within the peptide yields an inactive deriv. An abs. requirement for activation of the receptor is a 2nd-residue side chain of the appropriate size; analogs with 2nd-residue side chains too large or too small are inhibitory. On the basis of the activity of conformational analogs of glutathione, torsional angles for the 2nd residue equal to those of a right-handed .alpha.-helix are compatible with stimulus generation.

IT **82147-38-4**
(glutathione receptor of hydra interaction with, feeding behavior in relation to)

RN 82147-38-4 HCA

CN Glycine, L-.gamma.-glutamyl-1-aminocyclopentanecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 12-6 (Nonmammalian Biochemistry)

IT **Merrifield** synthesis
(of glutathione analogs)

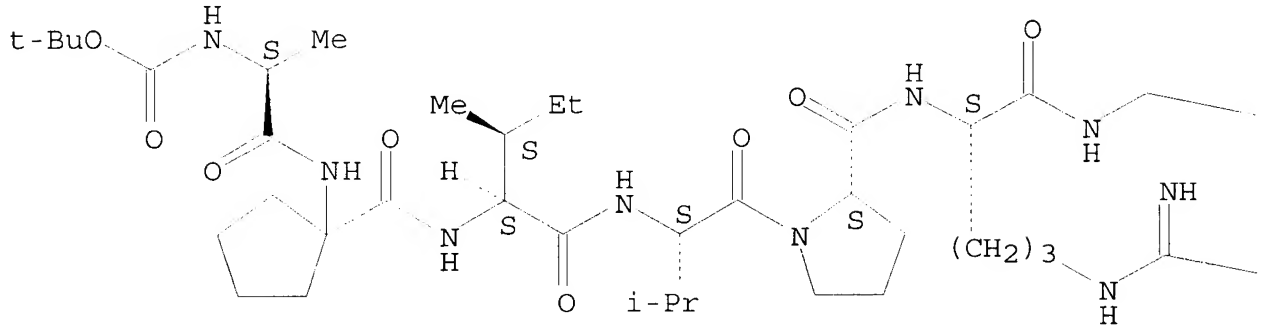
IT 52-90-4, biological studies 56-12-2, biological studies 56-40-6, biological studies 56-85-9, biological studies 56-86-0, biological studies 98-79-3 110-94-1 495-27-2 636-65-7 1948-48-7 2922-56-7 6600-40-4 13640-39-6 16305-88-7 27025-41-8 35989-16-3 38837-70-6 38837-71-7 38837-73-9 38837-74-0 71133-09-0 82147-32-8 82147-33-9 82147-34-0 82147-35-1 82147-36-2 82147-37-3 **82147-38-4** 82147-39-5 82147-40-8 82147-41-9 82147-42-0 82147-43-1 82147-44-2 82147-45-3 82147-46-4 82147-47-5 82147-48-6 82147-49-7 82147-50-0 82147-51-1 82147-52-2 82153-39-7

82153-40-0 82153-41-1 82153-42-2
(glutathione receptor of hydra interaction with, feeding behavior in relation to)
IT 57294-38-9P 68090-88-0P
(prepn. of, for **Merrifield** synthesis of glutathione analogs)

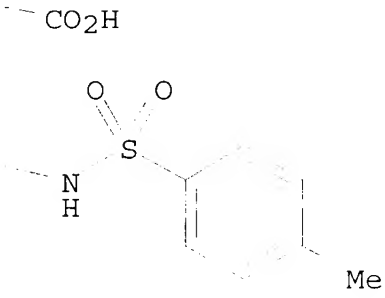
L27 ANSWER 15 OF 16 HCA COPYRIGHT 2003 ACS
97:6759 Enhancement of peptide coupling reactions by 4-dimethylaminopyridine. Wang, S. S.; Tam, J. P.; Wang, B. S. H.; Merrifield, R. B. (Peninsula Lab., Inc., Belmont, CA, USA). International Journal of Peptide & Protein Research, 18(5), 459-67 (English) 1981. CODEN: IJPPC3. ISSN: 0367-8377.
AB 4-Dimethylaminopyridine (DMAP) enhanced peptide coupling reactions which were mediated by DCC or sym. anhydrides. In an automated synthesis of Me3CO2C-Ala-Cle-Ile-Val-Pro-Arg(Tos)-Gly-OCH2-resin (Cle = cycloleucine residue, Tos = tosyl), the efficiencies of various coupling methods, e.g. as DCC, DCC/1-hydroxybenzotriazole, and sym. anhydride, were compared with that of DCC-DMAP. Only DCC-DMAP gave near quant. couplings in those cycles involving the sterically hindered amino acid residues. DMAP accelerated the sym. anhydride couplings in the synthesis of H-Leu-Ala-Gly-Val-OH. No racemization was detected during these couplings.
IT **81136-53-0DP**, resin-bound
(prepn. and resin cleavage of, by amidation)
RN 81136-53-0 HCA
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-1-aminocyclopentanecarbonyl-L-isoleucyl-L-valyl-L-prolyl-N5-[imino[[(4-methylphenyl)sulfonyl]amino]methyl]-L-ornithyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

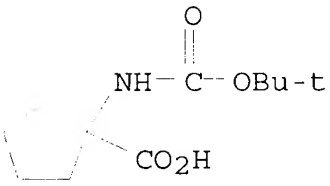
PAGE 1-A



PAGE 1-B



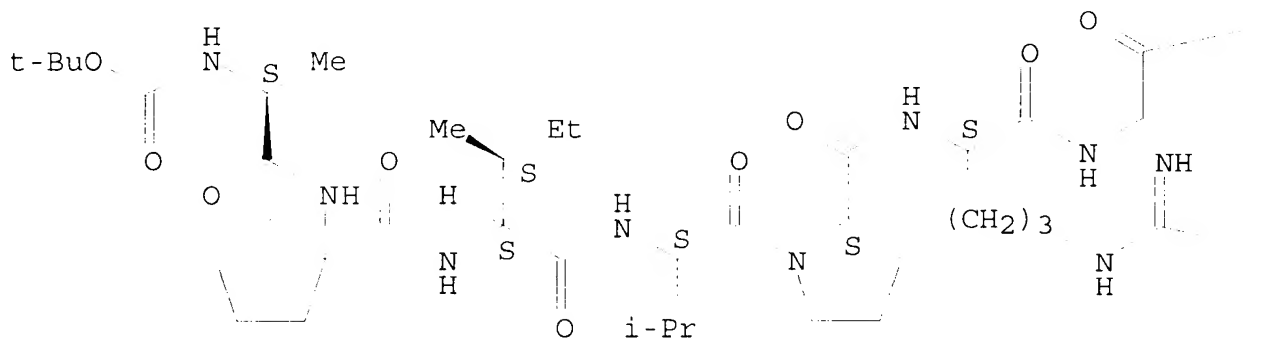
IT **35264-09-6P**
(prepn. and solid-phase peptide coupling of)
RN 35264-09-6 HCA
CN Cyclopentanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



IT **81136-54-1P**
(prepn. of, by solid-phase method, enhancement of peptide coupling reactions by dimethylaminopyridine in)
RN 81136-54-1 HCA
CN Glycinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-1-aminocyclopentanecarbonyl-L-isoleucyl-L-valyl-L-prolyl-N5-[imino[[(4-methylphenyl)sulfonyl]amino]methyl]-L-ornithyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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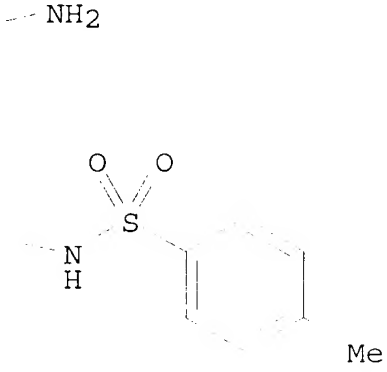
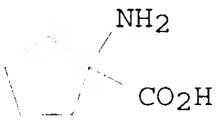


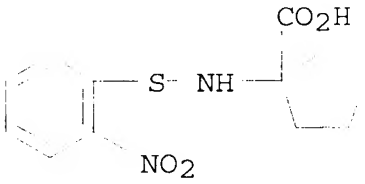
IT **52-52-8**
(tert-butoxycarbonylation of)
RN 52-52-8 HCA
CN Cyclopentanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 34-3 (Amino Acids, Peptides, and Proteins)
ST methylaminopyridine peptide coupling enhancement; peptide coupling enhancement dimethylaminopyridine; **Merrifield** synthesis dimethylaminopyridine enhancement; pyridine dimethylamino peptide coupling enhancement; DCC peptide coupling dimethylaminopyridine enhancement
IT **Merrifield** synthesis
(of peptides, dimethylaminopyridine for the enhancement of coupling reactions in)

IT **81136-53-0DP**, resin-bound
(prepn. and resin cleavage of, by amidation)
IT **35264-09-6P** 56676-12-1P
(prepn. and solid-phase peptide coupling of)
IT 79141-62-1P **81136-54-1P**
(prepn. of, by solid-phase method, enhancement of peptide coupling reactions by dimethylaminopyridine in)
IT **52-52-8**
(tert-butoxycarbonylation of)

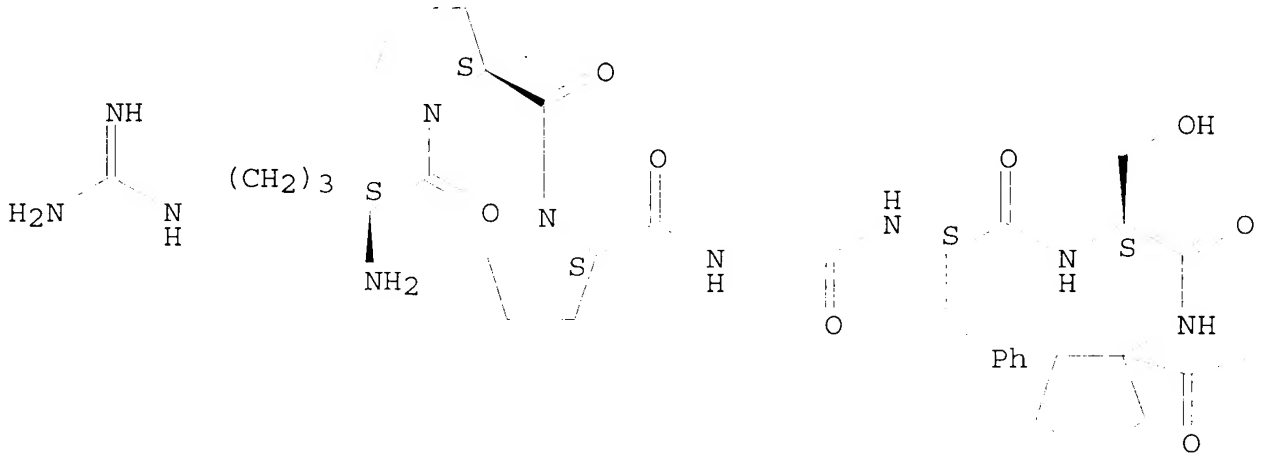
L27 ANSWER 16 OF 16 HCA COPYRIGHT 2003 ACS
89:24790 Synthesis of peptides by the solid-phase method. III. Bradykinin: fragments and analogs. Park, W. K.; St. Pierre, S. A.; Barabe, J.; Regoli, D. (Fac. Med., Univ. Sherbrooke, Sherbrooke, QC, Can.). Canadian Journal of Biochemistry, 56(2), 92-100 (English) 1978. CODEN: CJBIAE. ISSN: 0008-4018.
AB Bradykinin, Arg-Pro-Pro-Gly-Phe-Ser-Pro-Phe-Arg, and 55 fragments or analogs were prepd. by the solid-phase method and purified by ion-exchange and partition chromatog. The biol. activities of these peptides were tested in anesthetized cats (in vivo assay) and in rabbit aorta strips and cat ileum strips.
IT **46943-84-4**
(solid-phase peptide coupling of)
RN 46943-84-4 HCA
CN Cyclopentanecarboxylic acid, 1-[[(2-nitrophenyl)thio]amino]- (9CI) (CA INDEX NAME)



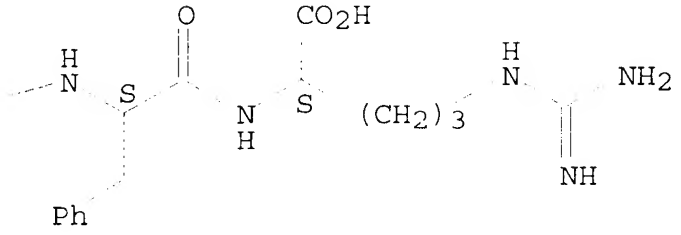
IT **67146-33-2**
(solid-phase prepn. and biol. activity of)
RN 67146-33-2 HCA
CN Bradykinin, 7-(1-aminocyclopentanecarboxylic acid)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 34-3 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 2
ST bradykinin analog **Merrifield**
IT **Merrifield** synthesis
(of bradykinin analogs)
IT 2188-18-3 4530-20-5 7764-95-6 13139-15-6 13139-16-7
13574-13-5 13734-34-4 15761-38-3 15761-39-4 18942-49-9
23680-31-1 37736-82-6 39608-31-6 **46943-84-4**
53267-93-9 57294-38-9
(solid-phase peptide coupling of)
IT 58-82-2 58-82-2D, analogs 3316-27-6 3322-87-0 3322-90-5

3322-91-6 5991-13-9 7379-22-8 7630-85-5 10318-24-8
14043-05-1 15024-88-1 15626-83-2 15958-92-6 16451-25-5
16511-76-5 16875-11-9 23815-85-2 23815-87-4 23815-88-5
23815-89-6 23842-74-2 25341-48-4 31021-87-1 32222-00-7
47917-73-7 51770-53-7 64695-06-3 64695-07-4 64695-08-5
64695-11-0 64695-12-1 64947-05-3 65431-73-4 65431-74-5
66582-61-4 66803-35-8 66803-36-9 66920-70-5 66920-71-6
66920-72-7 66920-73-8 66920-74-9 66976-61-2 66976-62-3
66976-63-4 66976-64-5 66976-65-6 66976-66-7 66976-67-8
66976-68-9 66976-69-0 66976-70-3 66976-71-4 66976-72-5
67146-33-2 67228-06-2
(solid-phase prepn. and biol. activity of)

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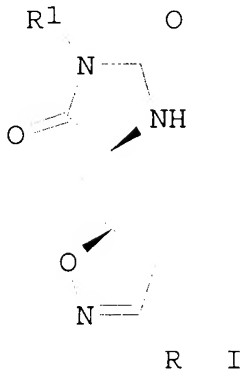
FILE 'HCA' ENTERED AT 13:22:03 ON 11 FEB 2003
L29 10052 SEA (SOLIDPHAS? OR SOLID?(3A)(PHASE# OR PHASING# OR SUPPORT?))(3A)(PREPAR? OR PREP# OR PREPN#)
L30 14358 SEA (POLYMER? OR RESIN?)(3A)BOUND?
L31 2640 SEA ((STAT# OR STATIONAR?)(3A)(PHASE# OR PHASING# OR SUPPORT?))(3A)(PREPAR? OR PREP# OR PREPN# OR SYN# OR SYNTH?)
L32 65 SEA L16 AND L29
L33 48 SEA L16 AND L30
L34 2 SEA L16 AND L31
L35 2 SEA L34 NOT L27
L36 99 SEA (L32 OR L33 OR L28) NOT (L27 OR L35)
L37 25 SEA L28 AND L32
L38 14 SEA L28 AND L33
L39 21 SEA L32 AND L33
L40 36 SEA (L37 OR L38 OR L39) NOT (L27 OR L35)
L41 63 SEA L36 NOT (L27 OR L35 OR L40)
L42 3 SEA L41 AND SOLID?/TI
L43 5 SEA L35 OR L42
L44 36 SEA L40 NOT L43
L45 60 SEA L41 NOT (L27 OR L43 OR L44)

=> d l43 1-5 cbib abs hitstr hitind

L43 ANSWER 1 OF 5 HCA COPYRIGHT 2003 ACS
134:71528 **Solid-phase synthesis** of novel achiral hydantoin- and isoxazoline-substituted dispirocyclobutanoids. Park, Kyung-Ho; Kurth, Mark J. (Dep. Chem., University of California, Davis, CA, 95616, USA). Chemical Communications (Cambridge) (19), 1835-1836 (English) 2000. CODEN: CHCOFS. ISSN: 1359-7345. OTHER SOURCES: CASREACT 134:71528. Publisher: Royal Society of Chemistry.
GI



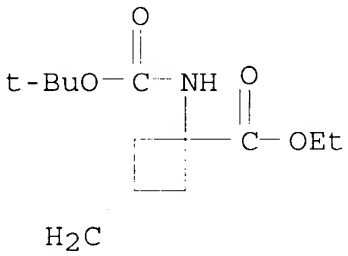
R I

AB A synthesis of novel achiral hydantoin- and isoxazoline-substituted dispirocyclobutanoids from **solid-phase synthesis** was achieved. The facial and selective Boc-NH-mediated H-bond delivery of a nitrile oxide afforded dispirocyclobutanoid I (R = Bz, Et; R1 = Ph, PhCH2, Bu) as the major compd.

IT **281207-62-3 313996-58-6**
(**solid-phase synthesis** of achiral hydantoin- and isoxazoline-substituted dispirocyclobutanoids)

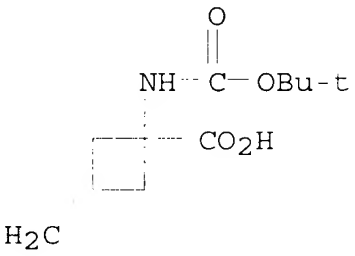
RN 281207-62-3 HCA

CN Cyclobutanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methylene-, ethyl ester (9CI) (CA INDEX NAME)



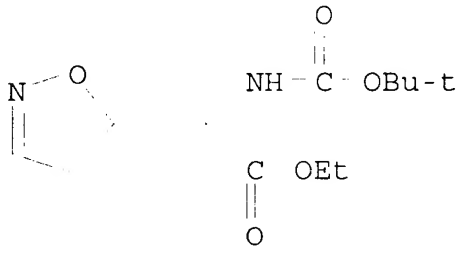
RN 313996-58-6 HCA

CN Cyclobutanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-3-methylene- (9CI) (CA INDEX NAME)

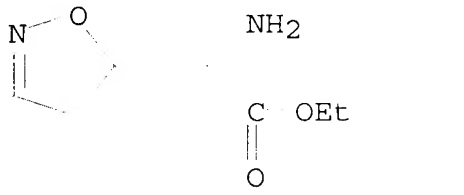


IT **313996-59-7P 313996-60-0P 313996-61-1P**
(**solid-phase synthesis** of achiral hydantoin- and isoxazoline-substituted dispirocyclobutanoids)

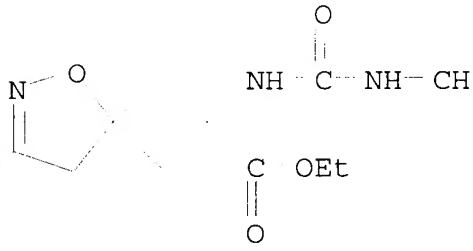
RN 313996-59-7 HCA
CN 5-Oxa-6-azaspiro[3.4]oct-6-ene-2-carboxylic acid, 2-[[(1,1-dimethylethoxy)carbonyl]amino]-7-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 313996-60-0 HCA
CN 5-Oxa-6-azaspiro[3.4]oct-6-ene-2-carboxylic acid, 2-amino-7-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 313996-61-1 HCA
CN 5-Oxa-6-azaspiro[3.4]oct-6-ene-2-carboxylic acid, 7-phenyl-2-[[[(phenylmethyl)amino]carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
ST isoxazoline hydantoin dispirocyclobutanoid **solid phase synthesis**
IT Spiro compounds
(**solid-phase synthesis** of achiral hydantoin- and isoxazoline-substituted dispirocyclobutanoids)

IT 103-71-9, Phenyl isocyanate, reactions 108-03-2, 1-Nitropropane 111-36-4, Butyl isocyanate 614-21-1, .alpha.-Nitroacetophenone 3173-56-6, Benzyl isocyanate **281207-62-3** **313996-58-6**
(**solid-phase synthesis** of achiral hydantoin- and isoxazoline-substituted dispirocyclobutanoids)

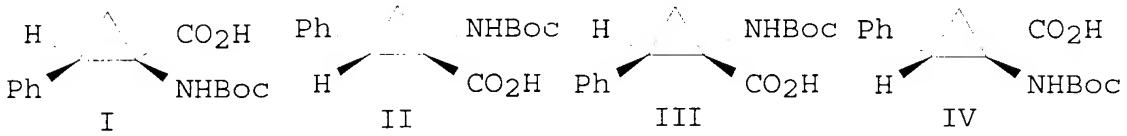
IT **313996-59-7P 313996-60-0P 313996-61-1P**
(**solid-phase synthesis** of achiral hydantoin- and isoxazoline-substituted dispirocyclobutanoids)

IT 282106-48-3P 314056-41-2P 314056-42-3P 314056-43-4P 314056-44-5P 314056-46-7P 314056-47-8P 314056-48-9P
(**solid-phase synthesis** of achiral hydantoin- and isoxazoline-substituted dispirocyclobutanoids)

L43 ANSWER 2 OF 5 HCA COPYRIGHT 2003 ACS

131:243549 Efficient access to all four stereoisomers of phenylalanine cyclopropane analogs by chiral HPLC. Cativiela, Carlos; Diaz-de-Villegas, Maria D.; Jimenez, Ana I.; Lopez, Pilar; Marraud, Michel; Oliveros, Laureano (Departamento de Quimica Organica, ICMA, Universidad de Zaragoza-CSIC, Zaragoza, 50009, Spain). Chirality, 11(7), 583-590 (English) 1999. CODEN: CHRLEP. ISSN: 0899-0042. Publisher: Wiley-Liss, Inc..

GI



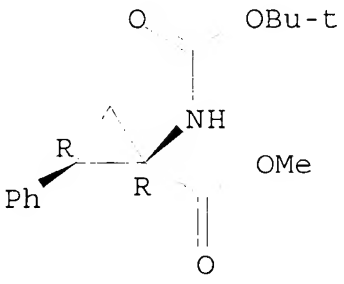
AB Bonded polysaccharide-derived chiral stationary phases were found to be useful for the prepn. of the four stereoisomers of phenylalanine cyclopropane (c3Phe) analogs I-IV as well as for the direct detn. of the enantiomeric purity of c3Phe derivs. by HPLC. Three chiral stationary phases, consisting of cellulose and amylose derivs. chem. bonded on allylsilica gel, were tested. The mixed 10-undecenoate/3,5-dimethylphenylcarbamate of cellulose, 10-undecenoate/3,5-dimethylphenylcarbamate of amylose and 10-undecenoate/p-methylbenzoate of cellulose were the starting polysaccharide derivs. for CSP-1 (CSP = chiral stationary phase), CSP-2, and CSP-3, resp. Using mixts. of n-hexane/chloroform/2-propanol as mobile phase on a semi-preparative column (150 mm .times. 20 mm ID) contg. CSP-2, the authors sepd. about 1.7 g of racemic Me cis-1-(tert-butoxycarbonyl)amino-2-phenylcyclopropanecarboxylate and 1.2 g of racemic Me trans-1-(tert-butoxycarbonyl)amino-2-phenylcyclopropanecarboxylate by successive injections.

IT **121079-69-4P 121096-91-1P 123039-88-3P 149666-26-2P 149666-27-3P 151910-10-0P 180322-78-5P 180322-80-9P 180322-85-4P**

197778-15-7P
(prepn. and sepn. of all four stereoisomers of phenylalanine cyclopropane analogs using HPLC with polysaccharide-derived chiral stationary phases)

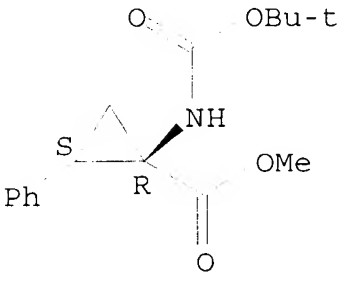
RN 121079-69-4 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, methyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



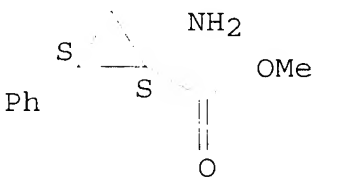
RN 121096-91-1 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, methyl ester, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



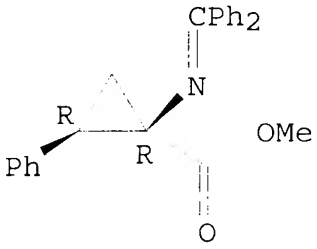
RN 123039-88-3 HCA
CN Cyclopropanecarboxylic acid, 1-amino-2-phenyl-, methyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



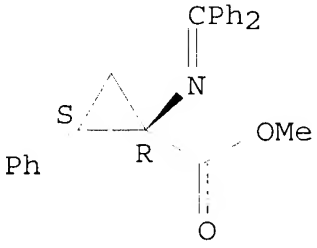
RN 149666-26-2 HCA
CN Cyclopropanecarboxylic acid, 1-[(diphenylmethylene)amino]-2-phenyl-, methyl ester, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



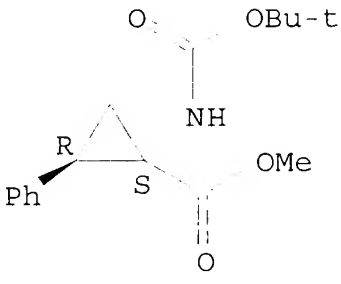
RN 149666-27-3 HCA
CN Cyclopropanecarboxylic acid, 1-[(diphenylmethylene)amino]-2-phenyl-, methyl ester, (1R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



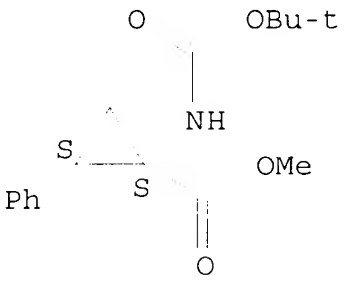
RN 151910-10-0 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, methyl ester, (1S,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



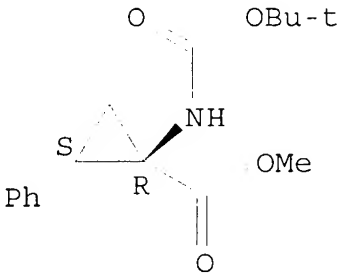
RN 180322-78-5 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, methyl ester, (1S,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



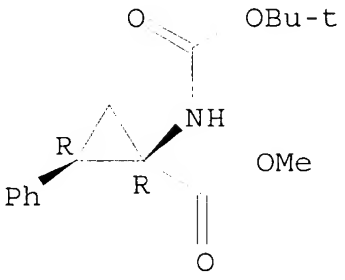
RN 180322-80-9 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, methyl ester, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



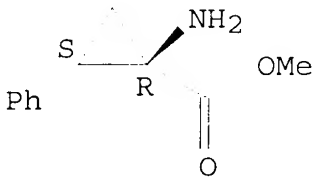
RN 180322-85-4 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, methyl ester, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 197778-15-7 HCA
CN Cyclopropanecarboxylic acid, 1-amino-2-phenyl-, methyl ester, (1R,2S)-rel- (9CI) (CA INDEX NAME)

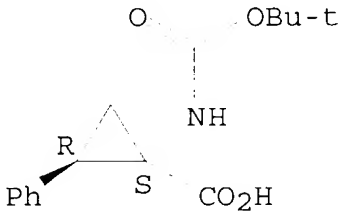
Relative stereochemistry.



IT **151910-11-1P 180322-79-6P 180322-86-5P 244205-60-5P**
(prepn. and sepn. of all four stereoisomers of phenylalanine cyclopropane analogs using HPLC with polysaccharide-derived chiral stationary phases)

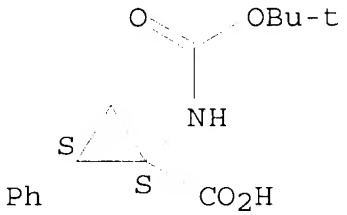
RN 151910-11-1 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, (1S,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



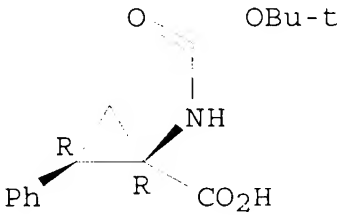
RN 180322-79-6 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, (1S,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



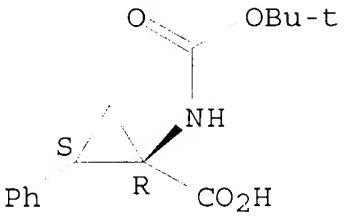
RN 180322-86-5 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 244205-60-5 HCA
CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-2-phenyl-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 80
IT HPLC **stationary phases**
(chiral; **prepn.** and sepn. of all four stereoisomers of phenylalanine cyclopropane analogs using HPLC with polysaccharide-derived chiral stationary phases)
IT **121079-69-4P 121096-91-1P 123039-88-3P**
149666-26-2P 149666-27-3P 151910-10-0P
180322-78-5P 180322-80-9P 180322-85-4P
197778-15-7P
(prepn. and sepn. of all four stereoisomers of phenylalanine cyclopropane analogs using HPLC with polysaccharide-derived chiral stationary phases)
IT **151910-11-1P 180322-79-6P 180322-86-5P**
244205-60-5P
(prepn. and sepn. of all four stereoisomers of phenylalanine cyclopropane analogs using HPLC with polysaccharide-derived chiral stationary phases)

L43 ANSWER 3 OF 5 HCA COPYRIGHT 2003 ACS
127:205857 N.alpha.-Fmoc-O,O-(dimethylphospho)-L-tyrosine fluoride: a convenient building block for the **solid-phase synthesis** of phosphotyrosyl peptides. Fretz, Heinz (Oncology Research, Novartis Pharma AG, Basel, CH-4002, Switz.). Letters in Peptide Science, 4(3), 171-176 (English) 1997. CODEN: LPSCEM. ISSN: 0929-5666. Publisher: Kluwer.
AB Fmoc-O,O-(dimethylphospho)-L-tyrosine, Fmoc-Tyr(PO3Me2)-OH, was

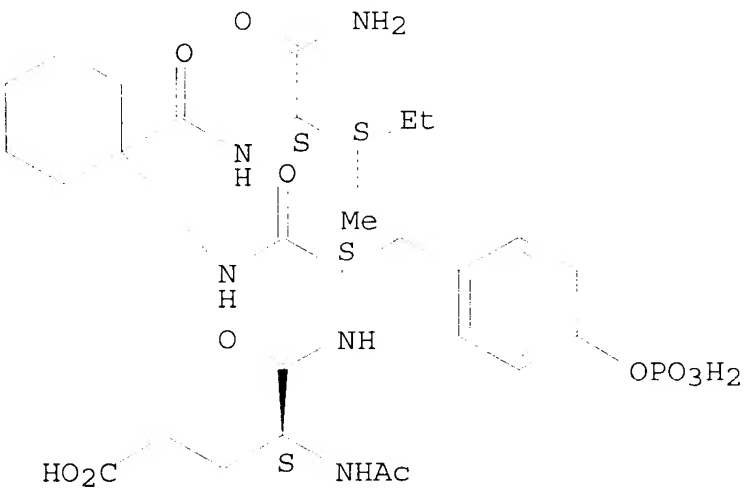
converted into stable Fmoc-O,O-(dimethylphospho)-L-tyrosine fluoride, Fmoc-Tyr(PO3Me2)-F, by means of (diethylamino)sulfur trifluoride or cyanuric fluoride. This building block was used for efficient coupling of phosphotyrosine to the adjacent sterically hindered amino acid Aib or Ac6c (Aib = .alpha.-aminoisobutyric acid, Ac6c = 1-aminocyclohexyl-1-carboxylic acid) in model peptide sequences as well as for the synthesis of the "difficult" phosphotyrosine peptide Stat91695-708. The phosphate Me groups were cleaved on solid phase after peptide assembly by means of trimethylsilyl iodide in MeCN.

IT **194592-61-5P**
(**solid-phase synthesis** of phosphotyrosyl peptides using (dimethylphospho)tyrosine fluoride)

RN 194592-61-5 HCA

CN L-Isoleucinamide, N-acetyl-L-.alpha.-glutamyl-O-phosphono-L-tyrosyl-1-aminocyclohexanecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 34-3 (Amino Acids, Peptides, and Proteins)

ST tyrosine fluoride dimethylphospho deriv prepn; phosphotyrosine peptide coupling aminoisobutyrate aminocyclohexylcarboxylate; peptide phosphotyrosyl **solid phase synthesis**

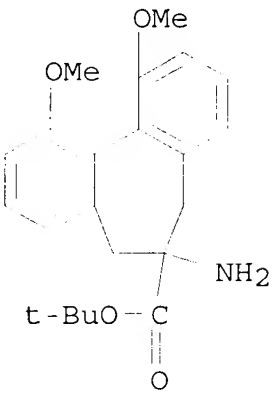
IT **Solid phase synthesis**
(peptide; **solid-phase synthesis** of phosphotyrosyl peptides using (dimethylphospho)tyrosine fluoride)

IT Phosphopeptides
(phosphotyrosine-contg.; **solid-phase synthesis** of phosphotyrosyl peptides using (dimethylphospho)tyrosine fluoride)

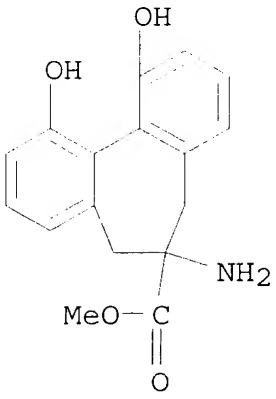
IT 127633-36-7 194592-59-1
(**solid-phase synthesis** of phosphotyrosyl peptides using (dimethylphospho)tyrosine fluoride)

IT 194592-58-0P
(**solid-phase synthesis** of
phosphotyrosyl peptides using (dimethylphospho)tyrosine fluoride)
IT 188045-96-7P 194592-60-4P **194592-61-5P** 194592-62-6P
(**solid-phase synthesis** of
phosphotyrosyl peptides using (dimethylphospho)tyrosine fluoride)

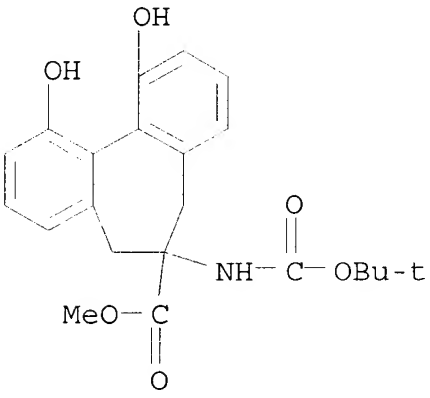
L43 ANSWER 4 OF 5 HCA COPYRIGHT 2003 ACS
126:305576 N-t-Boc-6-amino-1,11-(20-crown-6)-6,7-dihydro-5H-dibenzo[a,c]cycloheptene-6-carboxylic acid methyl ester, the first prototype of a crown-carrier-axially dissymmetric-.alpha.,.alpha.-disubstituted glycine. Mazaleyrat, Jean-Paul; Gaucher, Anne; Goubard, Yolaine; Savrda, Jaroslav; Wakselman, Michel (SIRCOB, Univ. Versailles, Versailles, 78000, Fr.). Tetrahedron Letters, 38(12), 2091-2094 (English) 1997. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier.
AB N-t-Boc-6-amino-1,11-(20-crown-6)-6,7-dihydro-5H-dibenzo[a,c]cycloheptene-6-carboxylic acid Me ester, a new crown-carrier-.alpha.,.alpha.-disubstituted glycine with axial dissymmetry and a potential building block for the synthesis of polypeptide supramol. devices, has been **synthesized** in the racemic **state** by **phase** transfer bisalkylation of a glycine tert-Bu ester Schiff case with 2,2'-bis(bromomethyl)-6,6'-dimethoxy-1,1'-biphenyl, followed by demethylation, esterification, N-protection and crown formation upon cyclization of the dicesium salt of the resulting diphenol with pentaethyleneglycol ditosylate.
IT **189232-22-2P 189232-24-4P 189232-26-6P**
(prepn. of a crown-carrier-axially dissym.-.alpha.,.alpha.-disubstituted glycine)
RN 189232-22-2 HCA
CN 5H-Dibenzo[a,c]cycloheptene-6-carboxylic acid, 6-amino-6,7-dihydro-1,11-dimethoxy-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



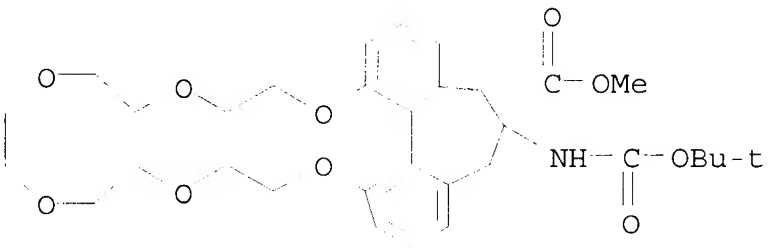
RN 189232-24-4 HCA
CN 5H-Dibenzo[a,c]cycloheptene-6-carboxylic acid, 6-amino-6,7-dihydro-1,11-dihydroxy-, methyl ester (9CI) (CA INDEX NAME)



RN 189232-26-6 HCA
CN 5H-Dibenzo[a,c]cycloheptene-6-carboxylic acid, 6-[[(1,1-dimethylethoxy)carbonyl]amino]-6,7-dihydro-1,11-dihydroxy-, methyl ester (9CI) (CA INDEX NAME)



IT **189232-19-7P**
(prepn. of a crown-carrier-axially dissym.-.alpha.,.alpha.-disubstituted glycine)
RN 189232-19-7 HCA
CN 19H-17,18-[1]Propen[1]yl[3]ylidenecyclohepta[rs]-1,4,7,10,13,16-benzohexaoxacycloeicosin-20-carboxylic acid, 20-[[(1,1-dimethylethoxy)carbonyl]amino]-2,3,5,6,8,9,11,12,14,15,20,21-dodecahydro-, methyl ester (9CI) (CA INDEX NAME)

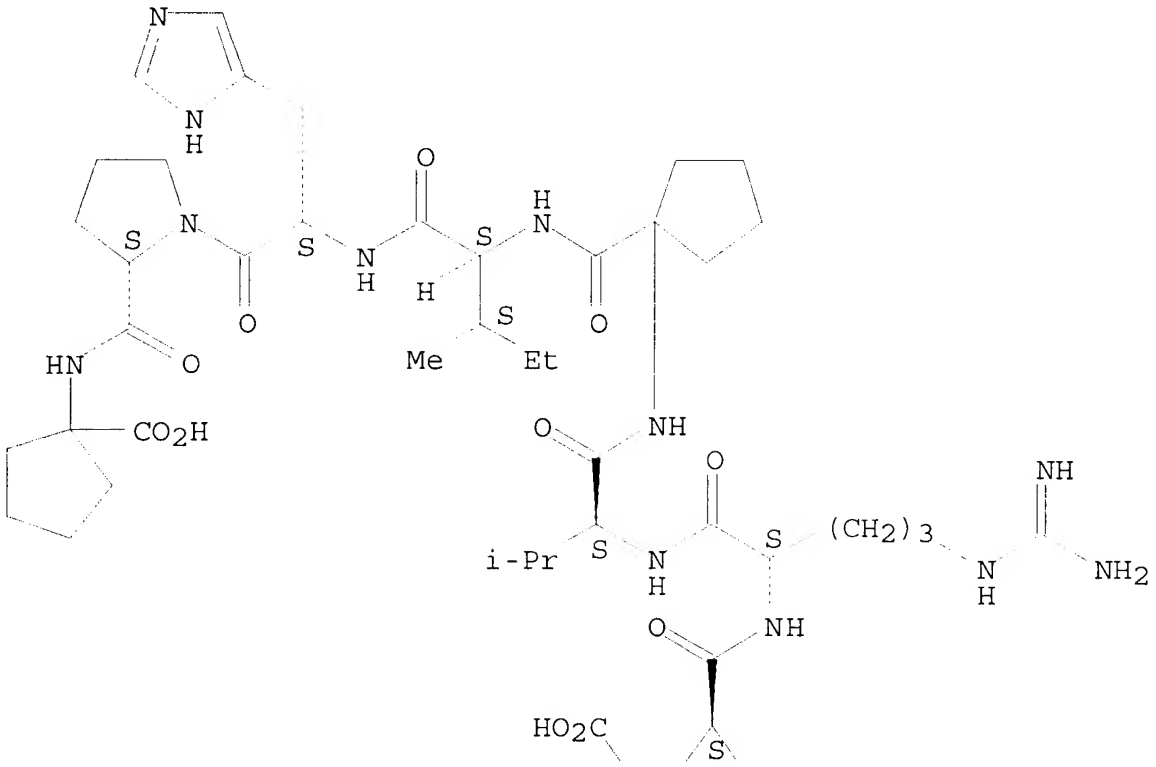


CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 34
IT **189232-22-2P 189232-24-4P 189232-26-6P**
(prepn. of a crown-carrier-axially dissym.-.alpha.,.alpha.-disubstituted glycine)
IT **189232-19-7P**
(prepn. of a crown-carrier-axially dissym.-.alpha.,.alpha.-disubstituted glycine)

L43 ANSWER 5 OF 5 HCA COPYRIGHT 2003 ACS
80:133794 Synthesis of peptides with the **solid** phase method. II. Octapeptide analogs of angiotensin II. Park, W. K.; Choi, C.; Rioux, F.; Regoli, D. (Dep. Pharmacol., Cent. Hosp. Univ., Sherbrooke, QC, Can.). Canadian Journal of Biochemistry, 52(2), 113-19 (English) 1974. CODEN: CJBIAE. ISSN: 0008-4018.
AB Forty-six analogs of angiotensin II were **prepd**. by **solid-phase** method. The peptides were purified using conventional procedures; homogeneity and purity were established by paper, thin-layer chromatog., paper electrophoresis, amino acid anal., elemental anal., and enzymatic degrdn. by aminopeptidase.
IT **52635-04-8P**
(prepn. of)
RN 52635-04-8 HCA
CN Angiotensin II, 4-(1-aminocyclopentanecarboxylic acid)-5-L-isoleucine-8-(1-aminocyclopentanecarboxylic acid)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

CC 34-3 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 2

IT 13761-29-0P 19729-18-1P 22684-01-1P 22684-02-2P 25119-43-1P
25157-97-5P 35463-61-7P 37574-65-5P 40678-47-5P 50725-20-7P
50725-21-8P 50725-22-9P 50725-23-0P 50765-42-9P 51833-69-3P
51833-70-6P 51833-72-8P 51833-73-9P 51833-74-0P 51833-76-2P
51887-62-8P 51887-64-0P 51887-65-1P 51887-66-2P 52634-92-1P
52634-93-2P 52634-94-3P 52634-95-4P 52634-96-5P 52634-97-6P
52634-98-7P 52634-99-8P 52635-00-4P 52635-01-5P 52635-02-6P
52635-03-7P **52635-04-8P** 52635-05-9P 52635-06-0P
52635-07-1P 52635-09-3P 52635-10-6P 52700-76-2P 52717-78-9P
52739-42-1P 52739-43-2P
(prepn. of)

=> d l44 1-36 cbib abs hitstr hitind

L44 ANSWER 1 OF 36 HCA COPYRIGHT 2003 ACS
137:385116 Preparation of vasoactive intestinal peptide analogs as anticancer agents. Burman, Anand C.; Prasad, Sudhanand; Mukherjee, Rama; Singh, Anu T.; Mathur, Archna; Gupta, Neena (Dabur Research Foundation, India). U.S. US 6489297 B1 20021203, 12 pp. (English). CODEN: USXXAM. APPLICATION: US 2000-630335 20000731.

AB Title peptides H-His-Ser-Asp-X1-Val-X2-Thr-Asp-Asn-Tyr-Thr-Arg-Leu-Arg-Lys-Gln-X3-Ala-Val-Lys-Lys-Tyr-Leu-Asn-Ser-Ile-Leu-Asn-NH2 (X1 = Aib, Deg, Ac5c; X2 = Phe, 4-Cl-D-Phe; R3 = Met, Leu, Dpg; Aib = .alpha.-aminoisobutyrate, Deg = .alpha.,.alpha.-diethylglycine, Ac5c = 1-aminocyclopentanecarboxyl; 4-Cl-D-Phe = 4-chloro-D-phenylalanyl; Dpg = .alpha.,.alpha.-di-n-propylglycine) contg. .alpha.,.alpha.-dialkyl amino acids in a site-specific manner were prepd. For example, H-His-Ser-Asp-Aib-Val-4-Cl-D-Phe-Thr-Asp-Asn-Tyr-Thr-Arg-Leu-Arg-Lys-Gln-Leu-Ala-Val-Lys-Lys-Tyr-Leu-Asn-Ser-Ile-Leu-Asn-NH2 (I) was **prepd.** via **solid-phase synthesis** using Fmoc-Asn(Trt)-resin and Fmoc chem. At 100 pM concn., I demonstrated the following percentage cytotoxicity values against specific tumor cell lines: 16 .+-. 3.3 (PA1, ovary), 16.9 .+-. 4.5 (SW620, colon), 10 .+-. 3.5 (HuTu80, duodenum), 18 .+-. 2.3 (L132, lung), 10.5 .+-. 4.5 (U87MG, glioblastoma), 47 .+-. 8.5 (KB, oral), 20 .+-. 6.5 (MIAPaCa2, pancreas), 16 .+-. 5.5 (A549, non-small cell lung), and 26 .+-. 5.5 (HT29, colon).

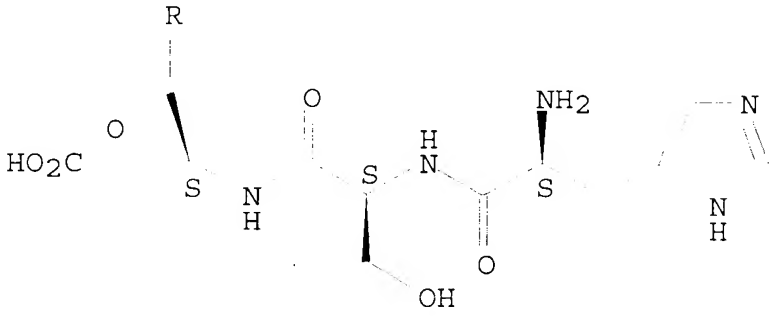
IT **355409-36-8P 355409-39-1P 355409-44-8P**
(prepn. and cytotoxicity activity of antitumor, vasoactive intestinal peptide analogs contg. site-specific dialkylated amino acids)

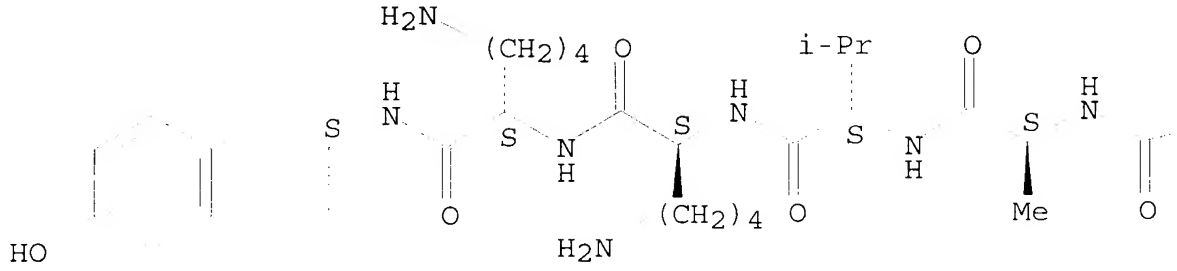
RN 355409-36-8 HCA

CN L-Aspartamide, L-histidyl-L-seryl-L-.alpha.-aspartyl-1-aminocyclopentanecarbonyl-L-valyl-4-chloro-D-phenylalanyl-L-threonyl-L-.alpha.-aspartyl-L-asparaginyl-L-tyrosyl-L-threonyl-L-arginyl-L-leucyl-L-arginyl-L-lysyl-L-glutaminyl-L-leucyl-L-alanyl-L-valyl-L-lysyl-L-lysyl-L-tyrosyl-L-leucyl-L-asparaginyl-L-seryl-L-isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





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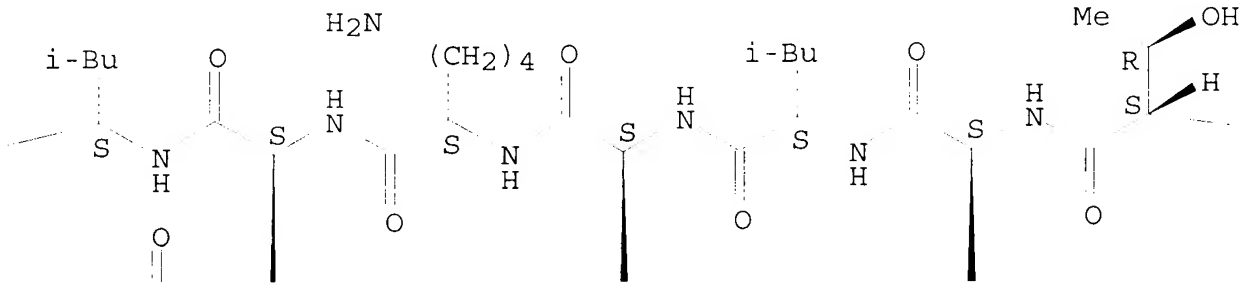

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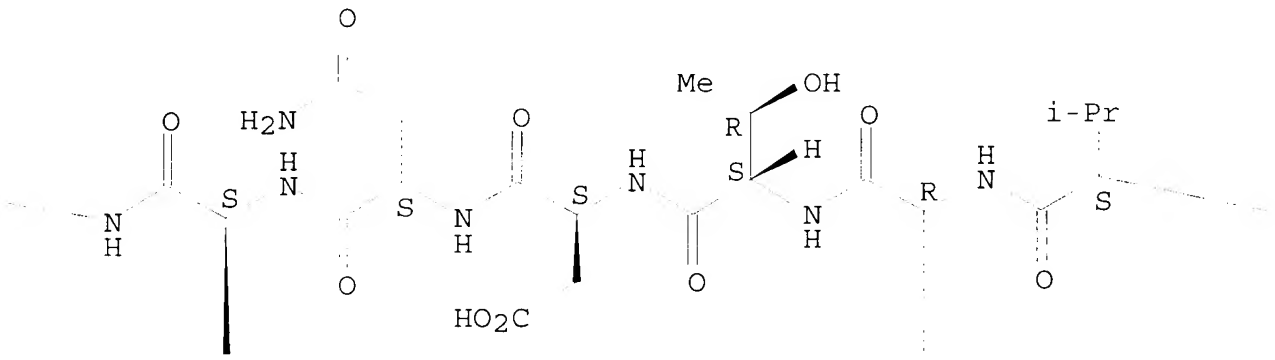

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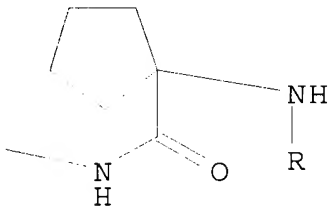

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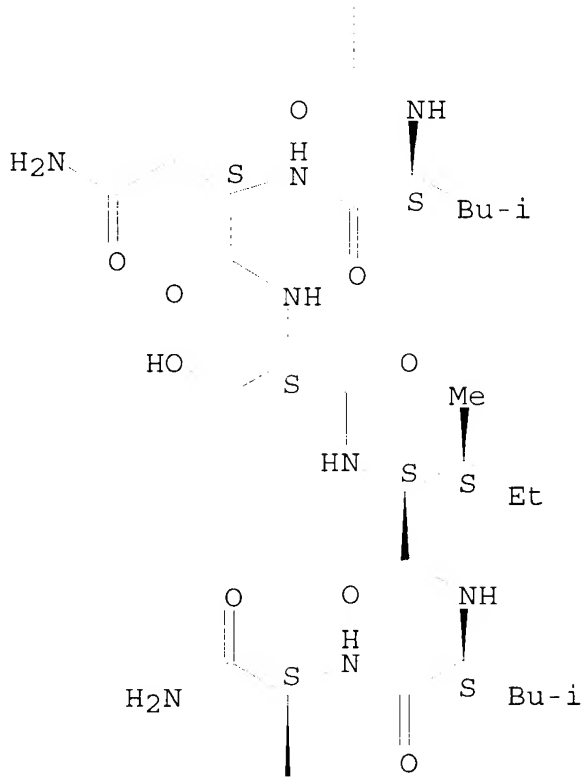

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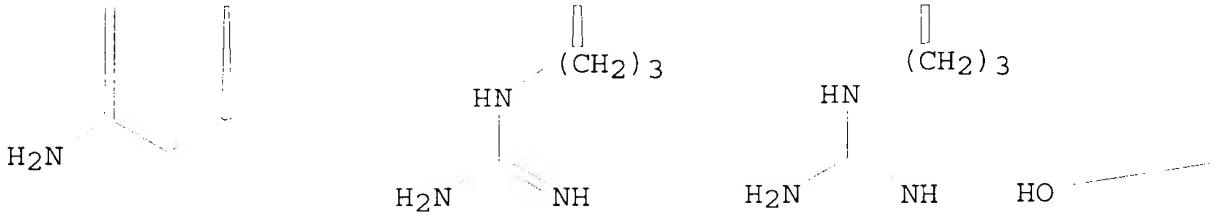

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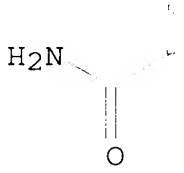

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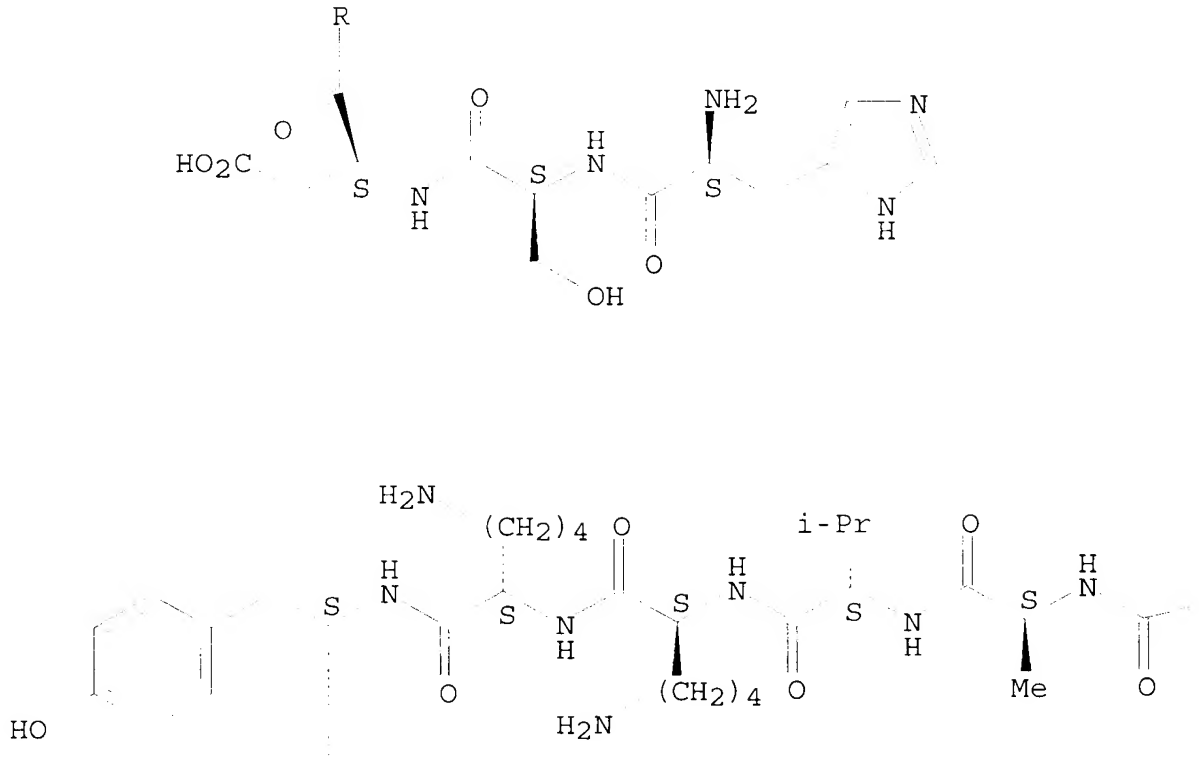
Absolute stereochemistry.

PAGE 1-A



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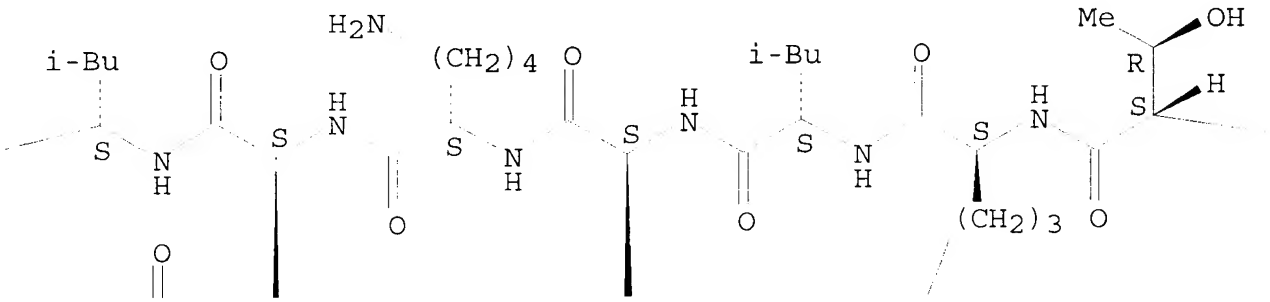

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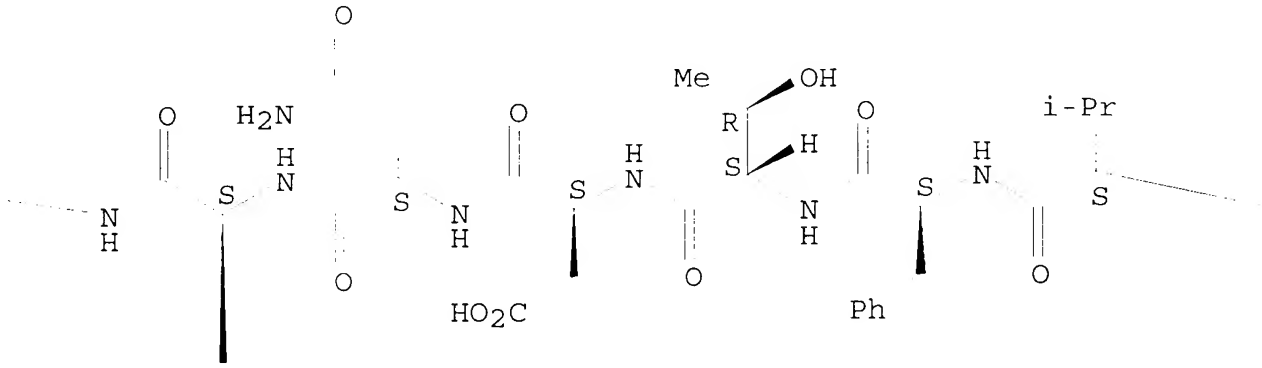

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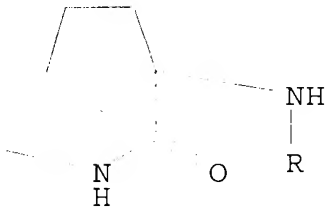

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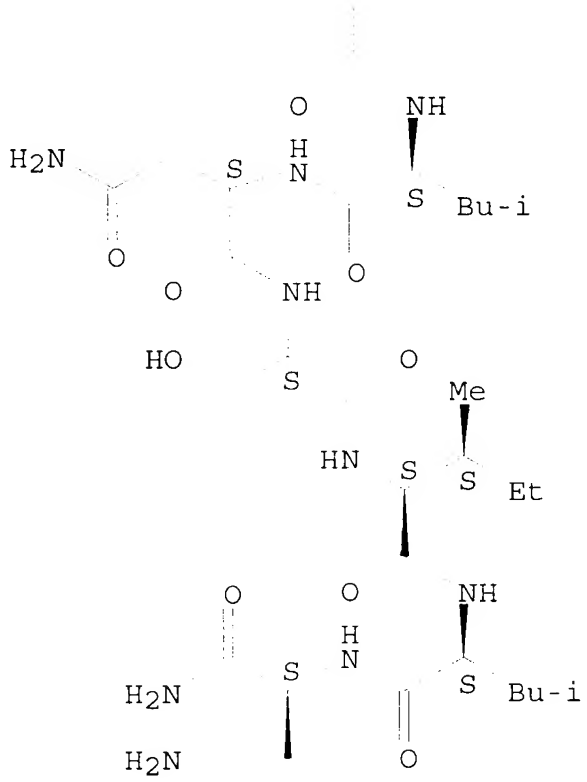

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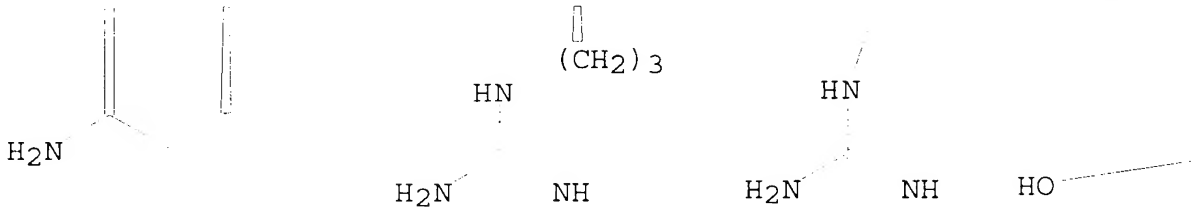

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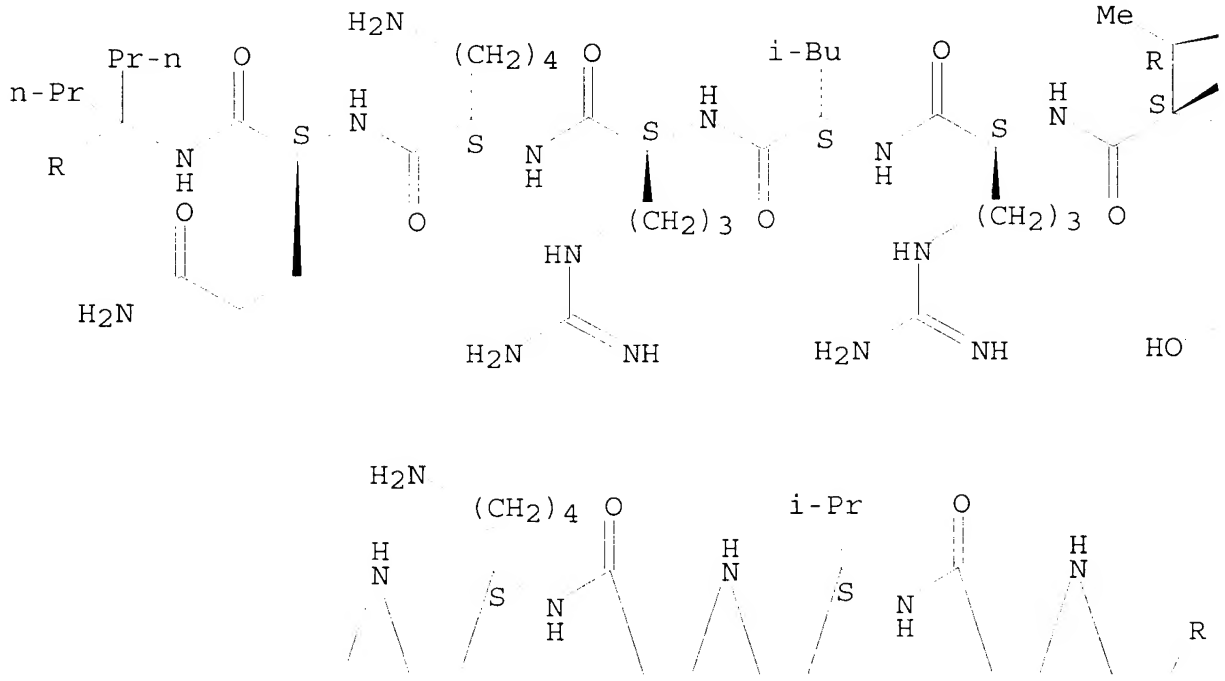
PAGE 3-A

RN 355409-44-8 HCA
CN L-Aspartamide, L-histidyl-L-seryl-L-.alpha.-aspartyl-1-aminocyclopentanecarbonyl-L-valyl-L-phenylalanyl-L-threonyl-L-.alpha.-aspartyl-L-asparaginyl-L-tyrosyl-L-threonyl-L-arginyl-L-leucyl-L-arginyl-L-lysyl-L-glutaminyl-2-propylnorvalyl-L-alanyl-L-valyl-L-lysyl-L-lysyl-L-tyrosyl-L-leucyl-L-asparaginyl-L-seryl-L-isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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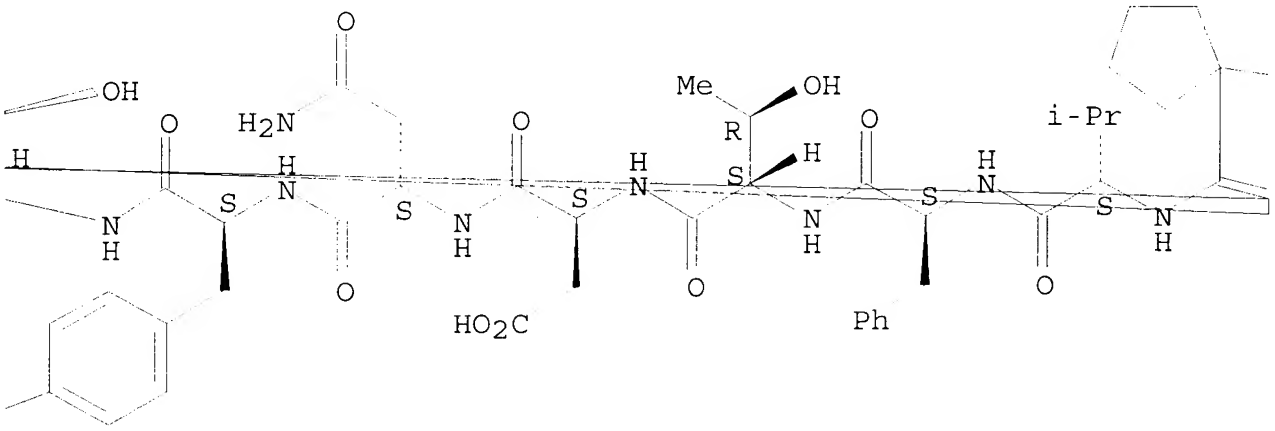

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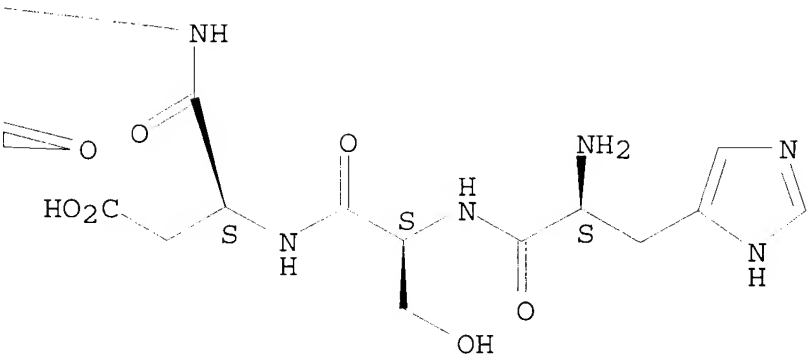

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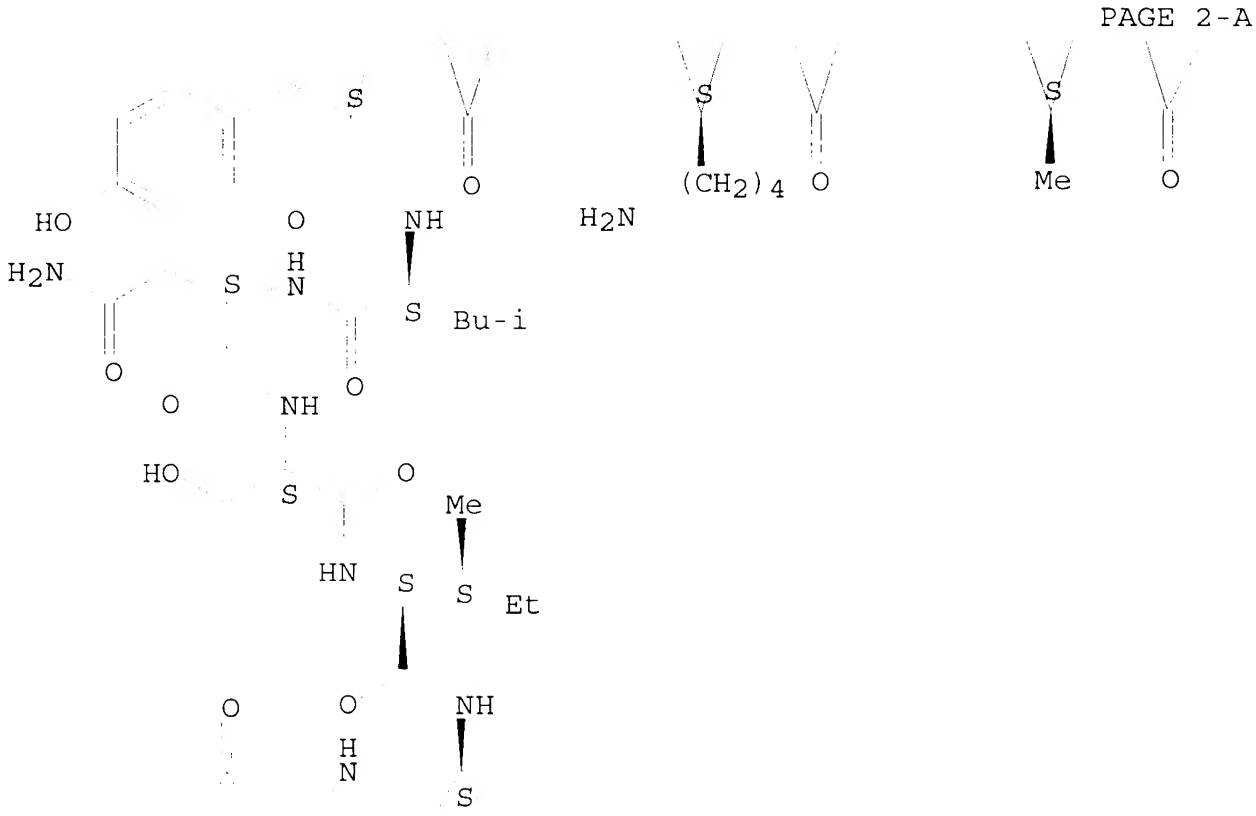

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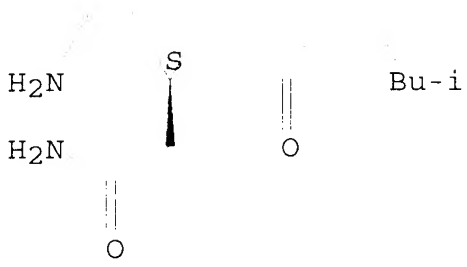


IT **52-52-8P**
(prepn. of dialkylated amino acids)
RN 52-52-8 HCA
CN Cyclopentanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

IC ICM A61K038-16
ICS C07K014-00
NCL 514012000; 530324000; 930170000
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1
IT 40077-57-4DP, Vasoactive intestinal octacosapeptide (swine), .alpha.,.alpha.-dialkyl amino acid-contg. analogs 355409-34-6P 355409-35-7P **355409-36-8P** 355409-37-9P 355409-38-0P **355409-39-1P** 355409-40-4P 355409-41-5P 355409-42-6P 355409-43-7P **355409-44-8P**
(prepn. and cytotoxicity activity of antitumor, vasoactive intestinal peptide analogs contg. site-specific dialkylated amino acids)
IT **52-52-8P**
(prepn. of dialkylated amino acids)

L44 ANSWER 2 OF 36 HCA COPYRIGHT 2003 ACS
137:295254 Preparation of peptide inhibitors of hepatitis C virus NS3 protease. Colarusso, Stefania; Gardelli, Cristina; Gerlach, Benjamin; Harper, Steven; Koch, Uwe; Matassa, Victor Giulio; Muraglia, Ester; Narjes, Frank; Ontoria, Ontoria Jesus Maria; Petrocchi, Alessia; Ponzi, Simona; Stansfield, Ian; Summa, Vincenzo (Istituto di Ricerche di Biologia Molecolare P. Angeletti Spa, Italy; et al.). PCT Int. Appl. WO 2002079234 A1 20021010, 151 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-EP3435 20020326. PRIORITY: GB 2001-7924 20010329.
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. I, II, and III [X = CH2, O; Y = CRa2, where Ra = H, OH, CO2H, alkyl, (hetero)aryl, (hetero)aralkyl, or CRa2 = cycloalkyl; Z = (un)substituted (hetero)aryl; R2 = alkyl, fluoroalkyl, or CH2SH; R3 = (un)substituted alkyl, (hetero)aryl, (hetero)aralkyl, or

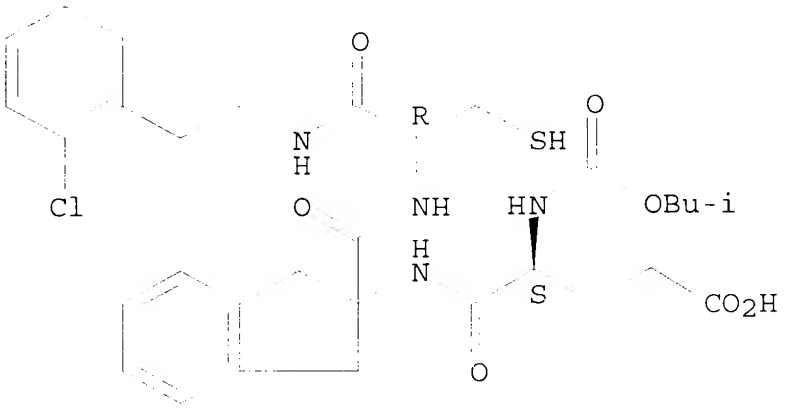
together with NRc forms a ring; Rc = H or alkyl or NRc together with R3 forms a ring; R4 = alkyl, alkenyl, (hetero)aralkyl, (hetero)aryl or an acidic group; R5 = (un)substituted carbamoyl, acyl, carboxylic ester, oxalyl, or sulfonyl group, which may be attached to an amino acid or a di- or tripeptide; R13 is a group contg. .ltoreq. 25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms and .ltoreq. 9 other heteroatoms which may be the same or different; R17 is H, alkyl, alkenyl, (hetero)aryl, (hetero)aralkyl, OH, alkoxy, aryloxy, (hetero)aralkoxy, thioether, sulfonyl or sulfoxide group; R18 is a group contg. .ltoreq. 25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms and .ltoreq. 9 other heteroatoms which may be the same or different] and their pharmaceutically-acceptable salts or esters were prepd. as inhibitors of the hepatitis C virus (HCV) NS3 protease. Thus, i-BuO2C-Glu-Leu-Cys-NHCH2CH2C6H3Cl2-2,4 was **prepd.** by the **solid-phase** method and showed IC50 .ltoreq. 10 .mu.M for inhibition of NS3 protease.

IT **467440-60-4P**
(prepn. of peptide inhibitors of hepatitis C virus NS3 protease)

RN 467440-60-4 HCA

CN L-Cysteinamide, N-[(2-methylpropoxy)carbonyl]-L-.alpha.-glutamyl-2-amino-2,3-dihydro-1H-indene-2-carbonyl-N-[2-(2-chlorophenyl)ethyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07K005-10
ICS C07K007-06

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7

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467441-09-4P 467441-10-7P 467441-11-8P 467441-12-9P
467441-13-0P
(prepn. of peptide inhibitors of hepatitis C virus NS3 protease)

IT 437-81-0P 637-59-2P, 1 Bromo 3 phenylpropane 935-42-2P
2417-72-3P 5162-82-3P, 3 Chloro 4 methylbenzoic acid 28229-69-8P
35303-76-5P 55304-25-1P 56161-89-8P 58971-11-2P 59311-67-0P,
3-Thiopheneethanamine 61048-76-8P 74733-30-5P 103201-78-1P
108052-76-2P 135248-89-4DP, **resin-bound**
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467438-37-5P 467438-38-6P 467438-39-7P 467438-40-0P
467438-41-1P 467438-42-2P 467438-43-3P 467438-44-4P
467438-45-5P 467438-46-6P 467438-50-2P 467438-51-3DP,
resin-bound 467438-52-4DP, **resin-**
bound 467438-53-5DP, **resin-bound**
467438-54-6DP, **resin-bound** 467438-56-8DP,
resin-bound 467438-57-9P 467438-58-0P
467438-59-1P 467438-60-4P 467438-61-5P 467438-62-6P
467438-63-7P 467438-64-8P 467438-65-9P 467438-66-0P
467438-67-1P 467438-68-2P 467438-70-6P 467438-71-7P
467438-72-8P 467438-73-9P 467442-04-2P 467442-05-3P
467442-06-4P 467442-07-5P 467442-08-6P 467442-09-7P
467442-10-0P 467442-11-1P 467442-12-2P 467442-13-3P
467442-14-4P 467442-15-5P 467442-16-6P 467442-17-7P
467442-18-8P 467442-19-9P 467442-20-2P 467442-21-3P
467442-22-4P 467442-23-5P 467442-24-6P 467442-25-7DP,
resin-bound 467442-26-8DP, **resin-**
bound 467442-28-0P 467442-29-1DP, **resin-**
bound 467442-30-4P 467442-34-8P 467442-35-9P
467442-36-0P 467442-37-1P 467442-38-2P
(prepn. of peptide inhibitors of hepatitis C virus NS3 protease)

L44 ANSWER 3 OF 36 HCA COPYRIGHT 2003 ACS
137:140770 A Novel Peptide-Based Encoding System for "One-Bead One-Compound" Peptidomimetic and Small Molecule Combinatorial Libraries. Liu, Ruiwu; Marik, Jan; Lam, Kit S. (Division of Hematology & Oncology Department of Internal Medicine, UC Davis Cancer Center University of California Davis, Sacramento, CA, 95817, USA). Journal of the American Chemical Society, 124(26), 7678-7680 (English) 2002. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The "one-bead one-compd." (OBOC) combinatorial library method is highly efficient, esp. when used with well-established on-bead binding or functional assays. Literally, millions of compds. can be screened concurrently within 1 to 2 days. However, structure detn. of peptidomimetic and small mol. compds. on one single bead is not trivial. A novel, highly efficient, and robust peptide-based encoding system has been developed for OBOC peptidomimetic and small mol. combinatorial libraries. In this system, topol. segregated

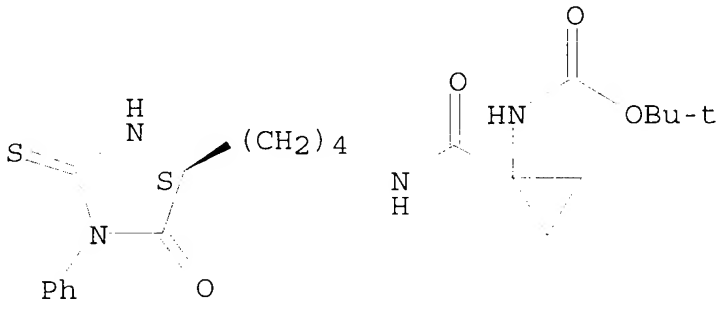
bifunctional beads, which are made by a simple biphasic solvent strategy, are employed for the prepn. and screening of an OBOC combinatorial peptidomimetic and small mol. libraries. Testing mols. are on the outer layer, and the coding tags in the interior of the bead do not interfere with screening. The coding tag is a peptide contg. a large no. of unnatural .alpha.-amino acids derived from different building blocks used for generating the peptidomimetic or small mol. By coupling common building blocks simultaneously to the scaffold of the testing compd. and to the side chains of the .alpha.-amino acids on the coding peptide, extra synthetic steps are eliminated and the amt. of undesirable side products is minimized. Pos. bead decoding is easy and straightforward as there is no need for cleavage and retrieval of the coding tag, and pos. beads can be sequenced directly with Edman degrdn. The authors demonstrate the efficiency and simplicity of their peptidyl encoding system by generating an encoded 158 400-member model peptidomimetic library and screening it for ligands that bind to streptavidin. Potent and novel ligands with clear motifs have been identified.

IT **444794-91-6**
(HPLC retention times of lysine phenylisothiocyanate derivs. used in the the encoding system for the "one-bead one-compd." combinatorial peptide library)

RN 444794-91-6 HCA

CN Carbamic acid, [1-[[[4-[(4S)-5-oxo-1-phenyl-2-thioxo-4-imidazolidinyl]butyl]amino]carbonyl]cyclopropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

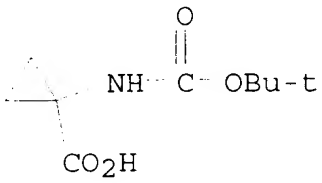
Absolute stereochemistry.



IT **88950-64-5**
(carboxylic acids and their derivs. used to derivatize aminophenylalanine and/or lysine in the encoding system for "one-bead one-compd." combinatorial peptide library)

RN 88950-64-5 HCA

CN Cyclopropanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 6

IT Amino acids, reactions
(N-[(fluorenylmethoxy)carbonyl]; **solid-phase prepn.** of a library of biol. active peptides using the "one-bead one-compd." combinatorial method, a novel peptide-based encoding system and a streptavidin-binding assay)

IT **Solid phase synthesis**
(combinatorial; **solid-phase prepn.** of a library of biol. active peptides using the "one-bead one-compd." combinatorial method, a novel peptide-based encoding system and a streptavidin-binding assay)

IT Peptide library
Peptidomimetics
(**solid-phase prepn.** of a library of biol. active peptides using the "one-bead one-compd." combinatorial method, a novel peptide-based encoding system and a streptavidin-binding assay)

IT Combinatorial chemistry
(**solid-phase; solid-phase prepn.** of a library of biol. active peptides using the "one-bead one-compd." combinatorial method, a novel peptide-based encoding system and a streptavidin-binding assay)

IT 444794-82-5 444794-83-6 444794-84-7 444794-85-8 444794-86-9
444794-87-0 444794-88-1 444794-89-2 444794-90-5
444794-91-6 444794-92-7 444794-93-8 444794-94-9
444794-95-0 444794-96-1 444794-97-2 444794-98-3 444794-99-4
444795-00-0 444795-01-1 444795-02-2 444795-03-3 444795-04-4
444795-06-6 444795-07-7 444795-08-8 444795-09-9 444795-10-2
444795-11-3 444795-12-4 444795-13-5 444795-14-6 444795-15-7
444795-16-8 444795-17-9 444795-18-0 444795-19-1 444795-20-4
444795-21-5 444795-22-6 444795-23-7 444795-24-8 444795-25-9
444795-26-0 444795-27-1 444795-28-2 444795-29-3 444795-30-6
444795-31-7 444795-32-8
(HPLC retention times of lysine phenylisothiocyanate derivs. used in the the encoding system for the "one-bead one-compd." combinatorial peptide library)

IT 65-85-0, Benzoic acid, reactions 79-09-4, Propionic acid, reactions 79-31-2, Isobutyric acid 86-87-3, 1-Naphthylacetic acid 88-13-1, 3-Thiophenecarboxylic acid 92-92-2, 4-Biphenylcarboxylic acid 98-79-3, L-Pyroglutamic acid 98-89-5, Cyclohexanecarboxylic acid 99-10-5, 3,5-Dihydroxybenzoic acid 99-64-9, 3-(Dimethylamino)benzoic acid 104-03-0,

4-Nitrophenylacetic acid 107-92-6, Butyric acid, reactions 108-55-4, Glutaric anhydride 116-53-0, 2-Methylbutyric acid 120-23-0, 2-Naphthoxyacetic acid 122-59-8, Phenoxyacetic acid 123-76-2, Levulinic acid 132-60-5, 2-Phenyl-4-quinolinecarboxylic acid 141-82-2, Malonic acid, reactions 142-62-1, Hexanoic acid, reactions 156-38-7, 4-Hydroxyphenylacetic acid 455-86-7, 3,4-Difluorobenzoic acid 499-06-9, 3,5-Dimethylbenzoic acid 501-52-0, Benzenepropanoic acid 527-72-0, 2-Thiophenecarboxylic acid 539-47-9, Furylacrylic acid 556-08-1, 4-Acetamidobenzoic acid 586-76-5, 4-Bromobenzoic acid 590-93-2, 2-Butynoic acid 619-84-1, 4-(Dimethylamino)benzoic acid 947-84-2, 2-Biphenylcarboxylic acid 1204-75-7, 3-Hydroxy-2-quinoxalinecarboxylic acid 1758-25-4, 2,5-Dimethoxyphenylacetic acid 1759-53-1, Cyclopropanecarboxylic acid 1877-73-2, 3-Nitrophenylacetic acid 1878-66-6, 4-Chlorophenylacetic acid 2067-33-6, 5-Bromovaleric acid 2215-77-2, 4-Phenoxybenzoic acid 2785-98-0, 2,5-Dimethoxybenzoic acid 2976-75-2, 1-Naphthoxyacetic acid 3535-37-3, 3,4-Dimethoxybenzoyl chloride 3724-19-4, 3-Pyridinepropionic acid 4282-31-9, 2,5-Thiophenedicarboxylic acid 4480-83-5, Diglycolic anhydride 4870-65-9, Bromophenylacetic acid 5427-26-9, 5-Hydantoinacetic acid 5807-30-7, 3,4-Dichlorophenylacetic acid 13794-14-4, 2-Phenoxybutyric acid 16534-12-6, 4-Bromo-3,5-dihydroxybenzoic acid 17078-28-3, 4-(Dimethylamino)phenylacetic acid 19337-97-4, trans-3-(3-Pyridyl)acrylic acid 19719-28-9, 2,4-Dichlorophenylacetic acid 29427-69-8, 3-Oxo-1-indanecarboxylic acid 33224-01-0, trans-4-Cotininecarboxylic acid 35718-08-2, Propargyl chloroformate 38496-18-3 39098-97-0, 2-Thiopheneacetyl chloride 41019-45-8, 5-(4-Chlorophenyl)-2-furoic acid 64362-32-9, 3-Benzoyl-2-pyridinecarboxylic acid **88950-64-5**
(carboxylic acids and their derivs. used to derivatize aminophenylalanine and/or lysine in the encoding system for "one-bead one-compd." combinatorial peptide library)

IT 9013-20-1, Streptavidin
(**solid-phase prepn.** of a library of biol. active peptides using the "one-bead one-compd." combinatorial method, a novel peptide-based encoding system and a streptavidin-binding assay)

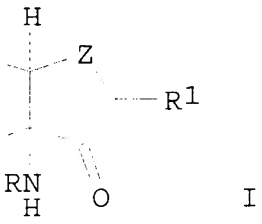
IT 444794-74-5P 444794-75-6P 444794-76-7P 444794-77-8P 444794-78-9P 444794-79-0P 444794-80-3P 444794-81-4P
(**solid-phase prepn.** of a library of biol. active peptides using the "one-bead one-compd." combinatorial method, a novel peptide-based encoding system and a streptavidin-binding assay)

IT 55-22-1, Isonicotinic acid, reactions 98-97-5, 2-Pyrazinecarboxylic acid 1477-50-5, Indole-2-carboxylic acid 29022-11-5, Fmoc-gly-OH 35661-60-0 71989-33-8 71989-38-3 95753-55-2 99333-54-7 119831-72-0 132388-59-1 157774-30-6 215190-27-5 444795-66-8, Boc-Lys(Dde)-OH
(**solid-phase prepn.** of a library of biol. active peptides using the "one-bead one-compd." combinatorial method, a novel peptide-based encoding system and a

streptavidin-binding assay)

L44 ANSWER 4 OF 36 HCA COPYRIGHT 2003 ACS
137:109484 Preparation of 1-aminocyclopentanecarboxylic acid-derived bicyclic compounds as inhibitors of cruzipain and other cysteine proteases. Quibell, Martin; Ramjee, Manoj Kumar (Incenta Limited, UK). PCT Int. Appl. WO 2002057246 A2 20020725, 118 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-GB194 20020117. PRIORITY: GB 2001-1204 20010117; US 2001-PV275506 20010313.

GI



I

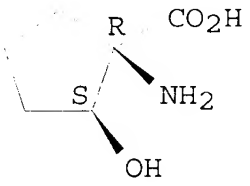
AB Title compds. I [R1 = H, alkyl, cycloalkyl, aryl, arylalkyl; Z = O, S, CR2R3 (R2, R3 is any group given for R1 or R1O, R1S, R1NH, R12N), or NR4 (R4-R11 is any group given for R1); R = U-Vm-Wn-Xm'-Y, where Y = CR5R6CO; X = CR7R8; W = O, S, CO, SO, SO2, NR9; V = CO, CS, SO, SO2, SO2NH, O2C, NHCO, NHSO, NHSO2, O2CNH, CONH, or CR10R11; m, m' = 0-3, n = 0 or 1; U = a stable 5- to 7-membered monocyclic or 8- to 11-membered bicyclic ring contg. 0-4 heteroatoms (provided that for m > 1, Vm contains a max. of one carbonyl or sulfonyl group)] were prepd. as inhibitors cruzipain (a gene product of Trypanosoma cruzi parasite) and other cysteine proteases for use as therapeutic agents, for example in the treatment of Chagas' disease. Thus, I (R1 = H, Z = O, R = p-tert-BuC6H4CO-Tyr) (II) was prepd. via intermediate (3aR,6aR)-[3-oxohexahydrocyclopenta[b]furan-3a-yl]carbamic acid 9H-fluoren-9-ylmethyl ester (8), which is available by a multistep procedure starting from cyclopentanone. Compd. 8 was attached to a linker and solid phase for coupling reactions with Fmoc-Tyr(OBut)-OH (Fmoc = fluorenylmethoxycarbonyl) and 4-tert-butylbenzoic acid. II was assayed for inhibition of cruzipain, bovine cathepsin S, and human cathepsins L and K (Ki = <2, >50, >20, and >100 .mu.M, resp.).

IT **197247-90-8P 443761-39-5P 443761-40-8P**
443761-41-9P 443761-42-0P 443761-43-1P

443761-44-2P
(prepn. of aminocyclopentanecarboxylic acid-derived bicyclic compds. as inhibitors of cruzipain and other cysteine proteases)

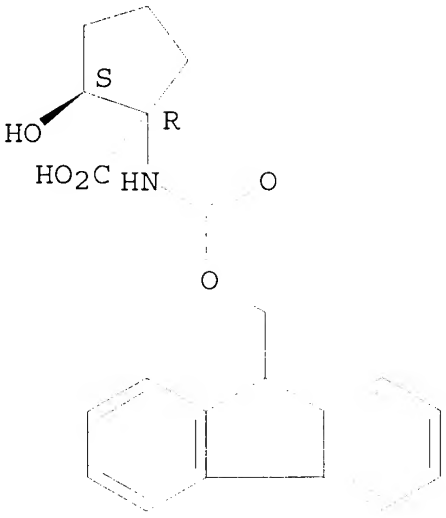
RN 197247-90-8 HCA
CN Cyclopentanecarboxylic acid, 1-amino-2-hydroxy-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



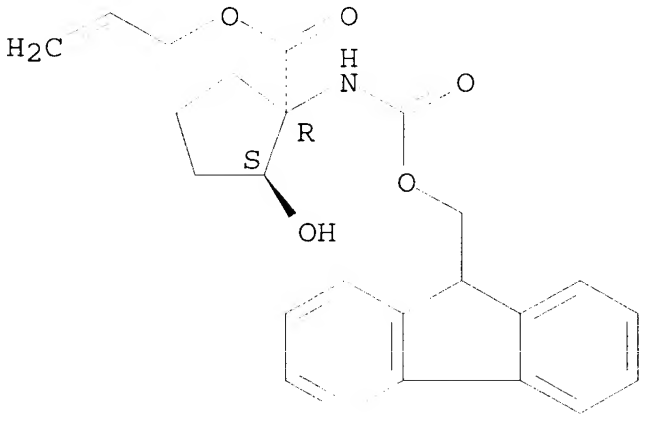
RN 443761-39-5 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-hydroxy-, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



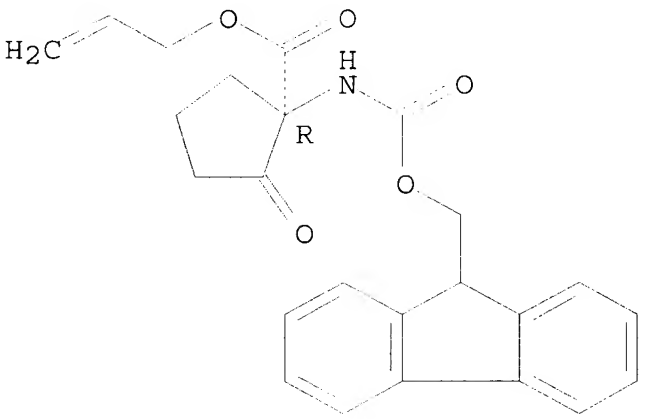
RN 443761-40-8 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-hydroxy-, 2-propenyl ester, (1R,2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



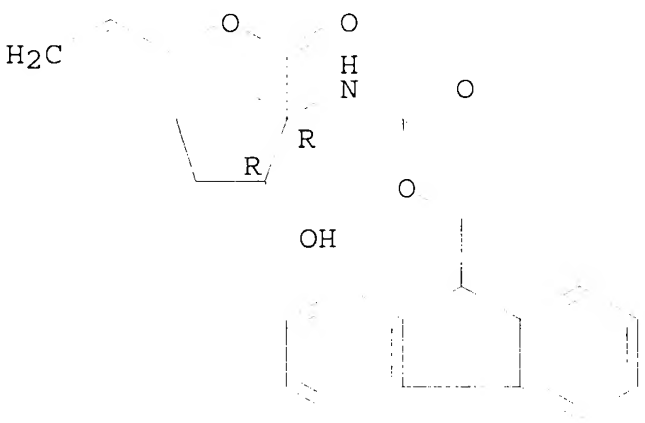
RN 443761-41-9 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-oxo-, 2-propenyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



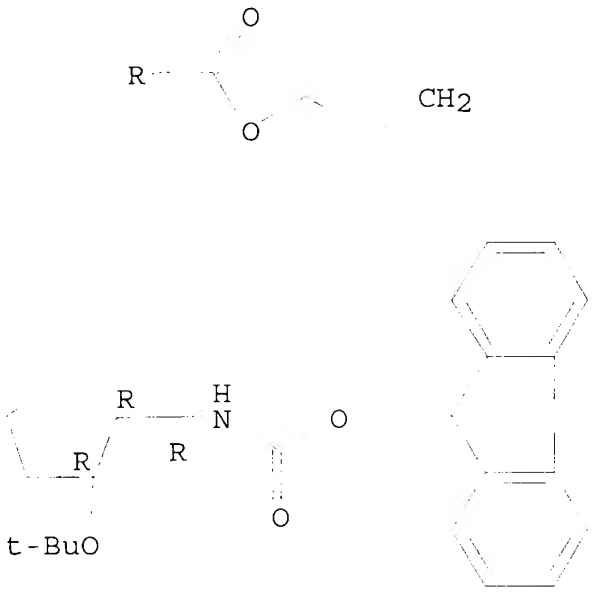
RN 443761-42-0 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-hydroxy-, 2-propenyl ester, (1R,2R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



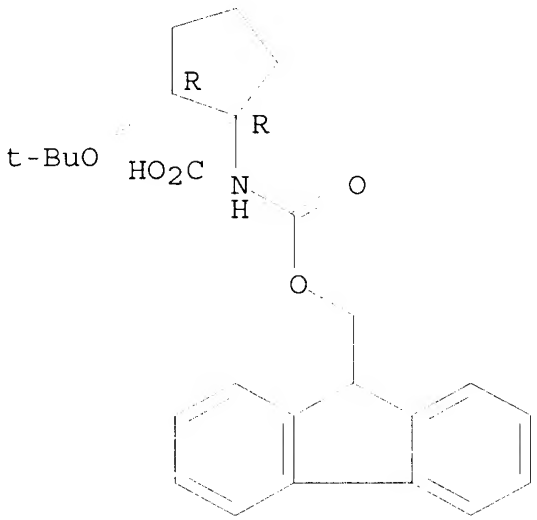
RN 443761-43-1 HCA
CN Cyclopentanecarboxylic acid, 2-(1,1-dimethylethoxy)-1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, 2-propenyl ester, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 443761-44-2 HCA
CN Cyclopentanecarboxylic acid, 2-(1,1-dimethylethoxy)-1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, (1R,2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07D307-00
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7, 24, 27
IT **Solid phase synthesis**
(peptide; **prepn.** of aminocyclopentanecarboxylic acid-derived bicyclic compds. as inhibitors of cruzipain and other cysteine proteases)
IT 23948-77-8P, [1,1'-Biphenyl]-3-acetic acid 42990-28-3P
62377-41-7P 63703-33-3P, 2,2-Dimethoxycyclopentanol 75852-28-7P
150529-73-0P 190661-70-2P 197247-75-9P 197247-76-0P
197247-78-2P **197247-90-8P** 215522-85-3P 324795-38-2P
324795-39-3P **443761-39-5P 443761-40-8P**
443761-41-9P 443761-42-0P 443761-43-1P
443761-44-2P 443761-45-3P 443761-46-4P 443761-47-5P
443761-48-6P 443761-61-3P 443761-62-4P
(prepn. of aminocyclopentanecarboxylic acid-derived bicyclic compds. as inhibitors of cruzipain and other cysteine proteases)

L44 ANSWER 5 OF 36 HCA COPYRIGHT 2003 ACS
137:109478 Synthesis and Biological Evaluation of Analogues of the Peptaibol Ampullosporin A. Nguyen, Hoai-Huong; Imhof, Diana; Kronen, Matthias; Schlegel, Brigitte; Haertl, Albert; Graefe, Udo; Gera, Lajos; Reissmann, Siegmund (Institut fuer Biochemie und Biophysik, Friedrich-Schiller-Universitaet Jena, Jena, D-07743, Germany). Journal of Medicinal Chemistry, 45(13), 2781-2787 (English) 2002. CODEN: JMCMAR. ISSN: 0022-2623. Publisher: American Chemical Society.
AB A series of analogs of the fungal peptaibol type metabolite ampullosporin A [Ac-Trp1-Ala-Aib-Aib-Leu-Aib-Gln-Aib-Aib-Aib-Gln-Leu-Aib-Gln-Leu15ol; Aib = .alpha.-aminoisobutyric acid, Leuol = leucinol] contg. modifications in the C and N terminus as well as Aib substitutions in different positions of the peptide were

synthesized by **solid-phase** methods using Fmoc chem. Depending on the sequence position, couplings were performed with HBTU/HOBt and PyBOP. The structures of the target peptides were analyzed by electrospray ionization mass spectrometry and chromatog. methods. The biol. activities of these peptides have been evaluated by assaying their potencies for the induction of pigment formation on the fungus Phoma destructiva as well as for the induction of hypothermia and inhibition of locomotoric activity in mice and were compared to those of the naturally occurring ampullosporins. Native ampullosporin A and analogs with C-terminal Leu or Leu-NH2 showed comparable activity in the pigmentation assay. Similarly, the ampullosporin A analogs with N-terminal arom. amino acid residues, such as D-Trp and Tic, also have high potency for pigment formation. The peptides contg. structural modifications of ampullosporin A by systematic replacement of Aib by Ala (Ala scan) displayed moderate or high activity in the pigmentation assay, whereas simultaneous substitution of all Aib residues by Ala and Ile, resp., or by insertion of nonarom. residues into position 1 resulted in a loss of the effect on P. destructiva. Most of the compds. with no or weak activity in the microbial assay were not active in the hypothermic test, too, except the peptide with 1-amino-1-cyclohexane carboxylic acid in position 4 instead of Aib. However, only a few peptides with high potency for pigmentation induction were found to produce strong hypothermia in mice.

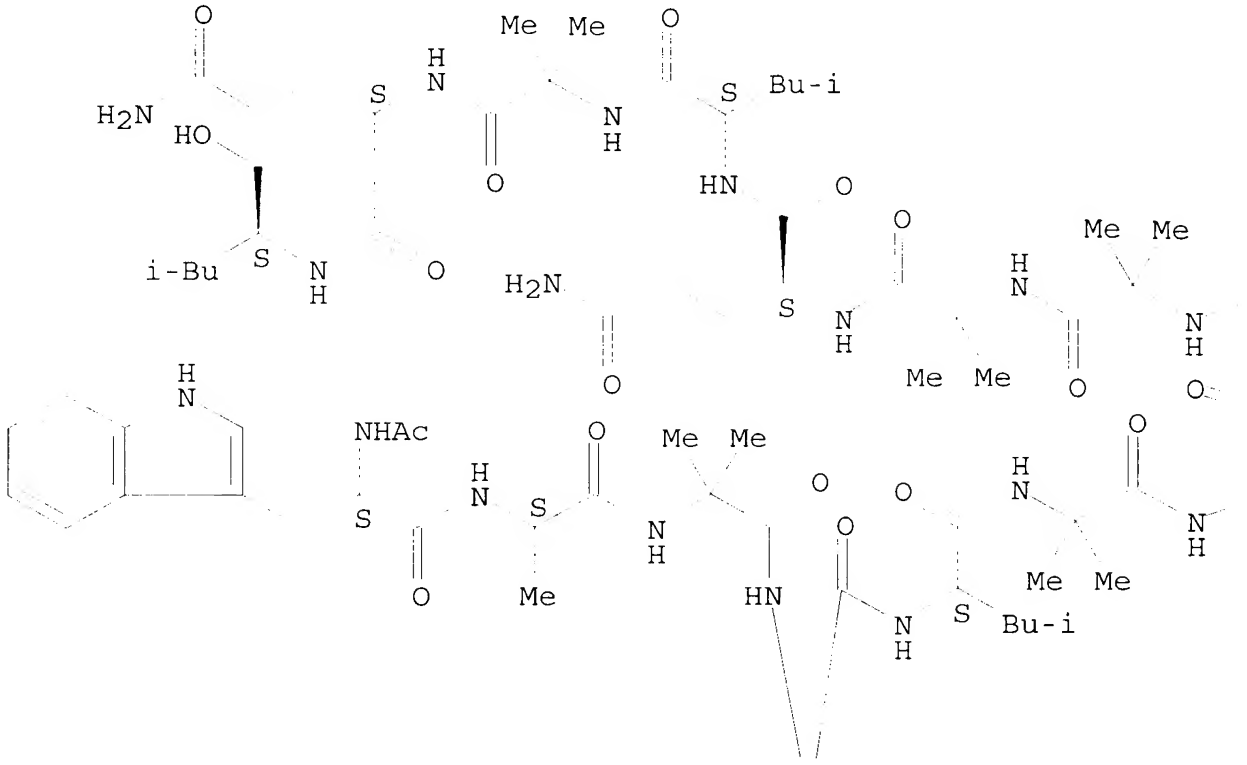
IT **442863-56-1P**
(**solid-phase synthesis** of ampullosporin analogs and their effects on reflex actions, locomotoric activity and body temps. in mice)

RN 442863-56-1 HCA

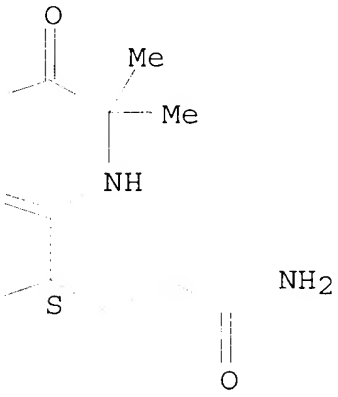
CN L-Glutamamide, N-acetyl-L-tryptophyl-L-alanyl-2-methylalanyl-1-aminocyclohexanecarbonyl-L-leucyl-2-methylalanyl-L-glutaminyl-2-methylalanyl-2-methylalanyl-2-methylalanyl-L-glutaminyl-L-leucyl-2-methylalanyl-N1-[(1S)-1-(hydroxymethyl)-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

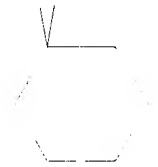
PAGE 1-A



PAGE 1-B



PAGE 2-A



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 10

ST peptaibol ampullosporin analog **solid phase** **prepn** biol evaluation; locomotoric activity structure relationship ampullosporin analog; hypothermia induction structure relationship ampullosporin analog

IT Peptides, **preparation**
(peptaibols; **solid-phase synthesis** of ampullosporin analogs and their effects on reflex actions, locomotoric activity and body temps. in mice)

IT **Solid phase synthesis**
(peptide; **solid-phase synthesis** of ampullosporin analogs and their effects on reflex actions, locomotoric activity and body temps. in mice)

IT Hypothermia
Muscle relaxants
Structure-activity relationship

Tranquilizers
(**solid-phase synthesis** of
ampullosporin analogs and their effects on reflex actions,
locomotoric activity and body temps. in mice)

IT 197960-94-4P, Ampullosporin A 338991-76-7P, Ampullosporin B
339075-00-2P, Ampullosporin C 339075-01-3P, Ampullosporin D
438042-57-0P 442863-41-4P 442863-42-5P 442863-43-6P
442863-44-7P 442863-45-8P 442863-46-9P 442863-47-0P
442863-48-1P 442863-49-2P 442863-50-5P 442863-51-6P
442863-52-7P 442863-53-8P 442863-54-9P 442863-55-0P
442863-56-1P 442863-57-2P 442863-58-3P
(**solid-phase synthesis** of
ampullosporin analogs and their effects on reflex actions,
locomotoric activity and body temps. in mice)

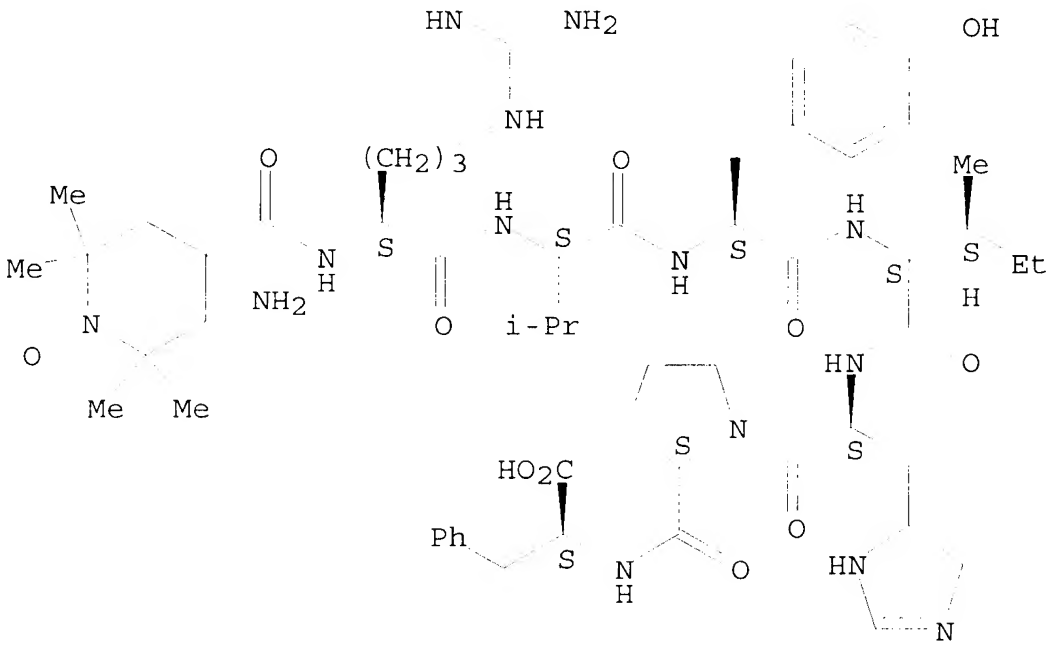
L44 ANSWER 6 OF 36 HCA COPYRIGHT 2003 ACS
136:355452 Synthesis and pharmacological properties of TOAC-labeled angiotensin and bradykinin analogs. Nakaie, C. R.; Silva, E. G.; Cilli, E. M.; Marchetto, R.; Schreier, S.; Paiva, T. B.; Paiva, A. C. M. (Department of Biophysics, Universidade Federal de Sao Paulo, Sao Paulo, SP, 04023-062, Brazil). Peptides (New York, NY, United States), 23(1), 65-70 (English) 2002. CODEN: PPTDD5. ISSN: 0196-9781. Publisher: Elsevier Science Inc..

AB Angiotensin II (AngII) and bradykinin (BK) derivs. contg. the TOAC (2,2,6,6-tetramethylpiperidine-N-oxyl-4-amino-4-carboxylic acid) spin label were **synthesized** by **solid phase** methodol. Ammonium hydroxide (pH 10, 50.degree.C, 1 h) was the best means for reverting nitroxide protonation occurring during peptide cleavage. EPR spectra yielded rotational correlation times for internally labeled analogs that were nearly twice as large as those of N-terminally labeled analogs. Except for TOAC1-AngII and TOAC0-BK, which showed high intrinsic activities, other derivs. were inactive in smooth muscle prepns. These active paramagnetic analogs may be useful for conformational studies in soln. and in the presence of model and biol. membranes.

IT **84606-48-4P 215931-15-0P**
(**solid phase** peptide **synthesis** and
smooth muscle contraction activity of paramagnetic spin-labeled
angiotensin and bradykinin analogs)

RN 84606-48-4 HCA
CN Angiotensin III, N2-[(4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinyl)carbonyl]-4-L-isoleucine- (9CI) (CA INDEX NAME)

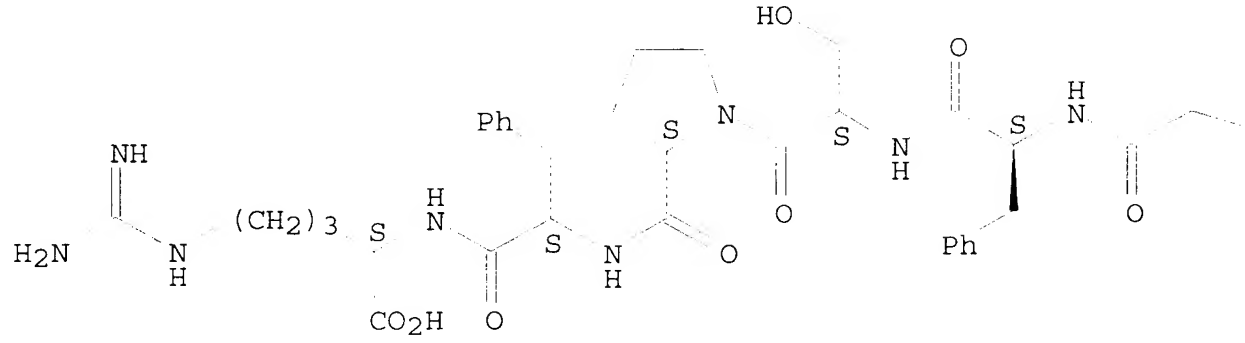
Absolute stereochemistry.



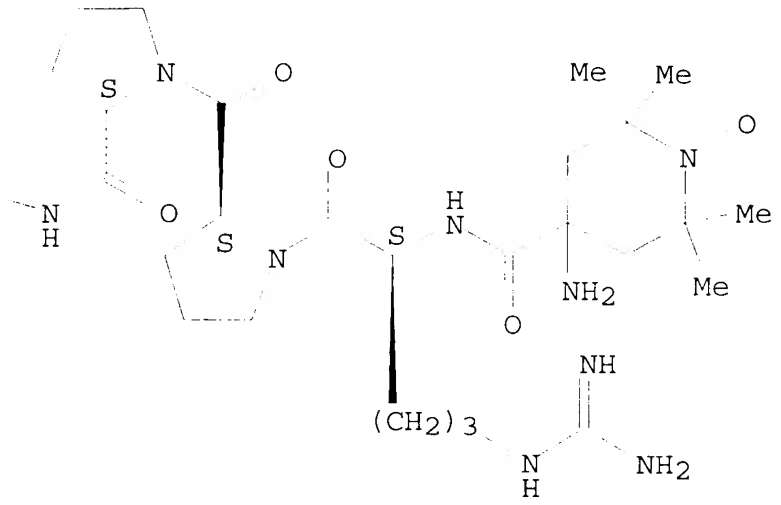
RN 215931-15-0 HCA
CN Bradykinin, N2-(4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

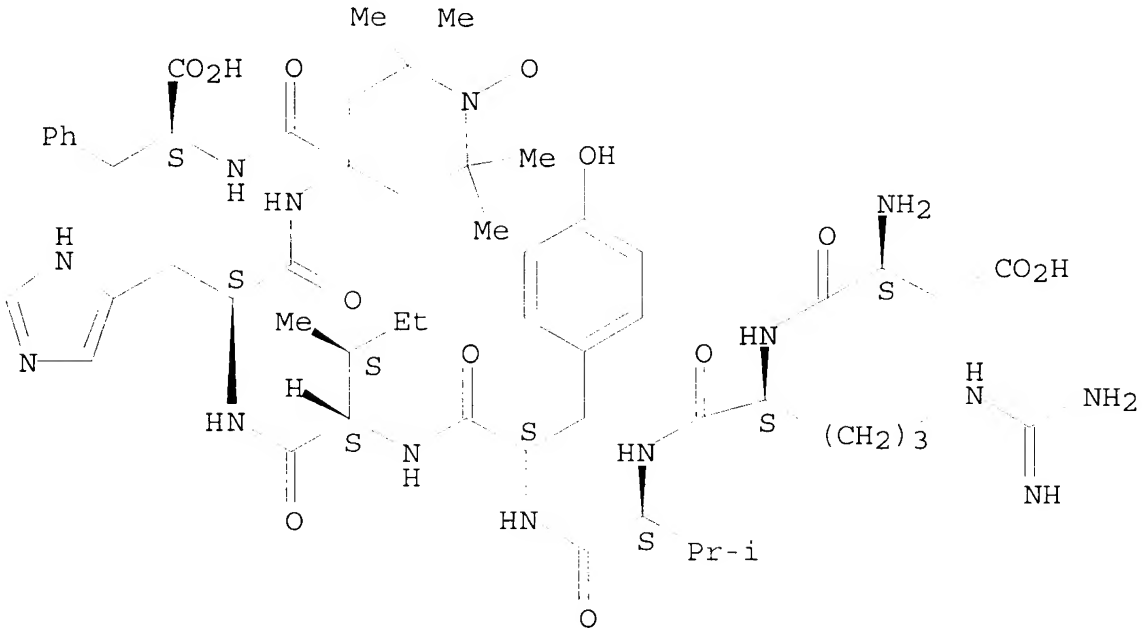


PAGE 1-B



IT **151842-58-9P 215931-19-4P 420819-95-0P**
(**solid phase** peptide **synthesis** and
smooth muscle contraction activity of paramagnetic spin-labeled
angiotensin and bradykinin analogs)
RN 151842-58-9 HCA
CN Angiotensin II, 5-L-isoleucine-7-(4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarboxylic acid)- (9CI) (CA INDEX NAME)

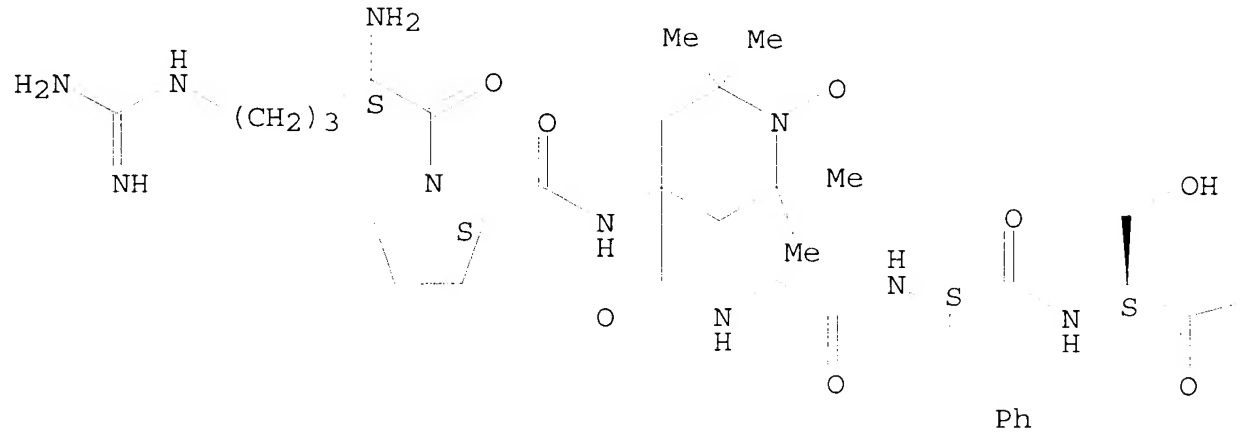
Absolute stereochemistry.



RN 215931-19-4 HCA
CN Bradykinin, 3-(4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarboxylic acid)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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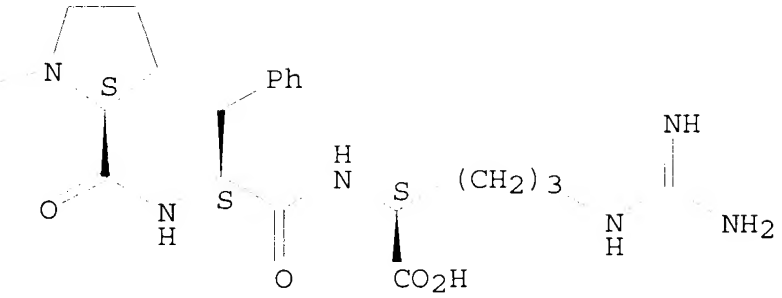
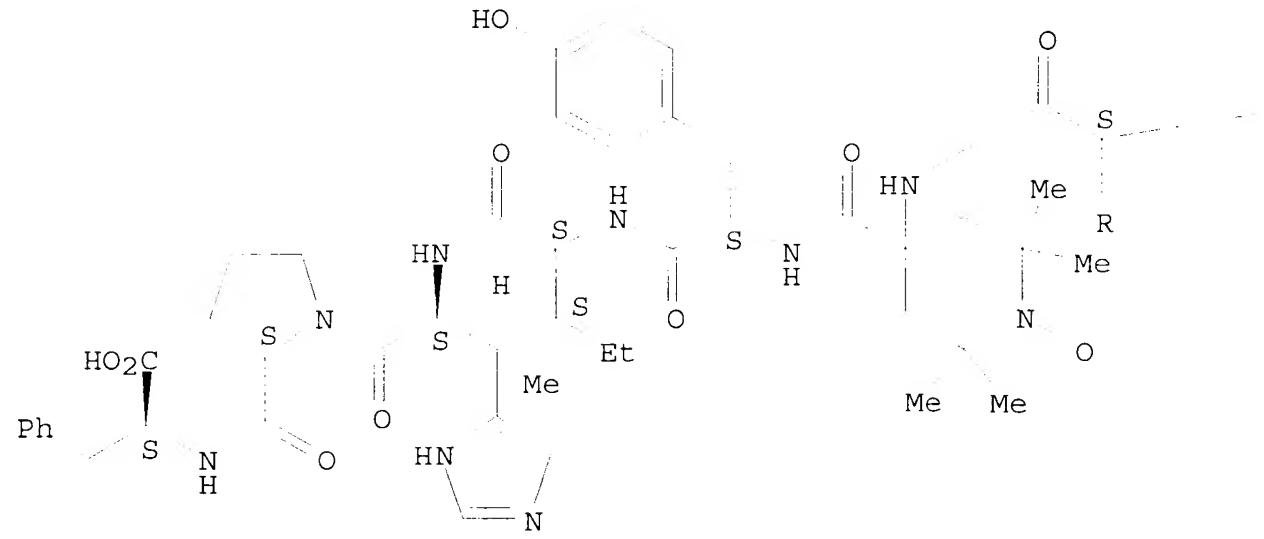


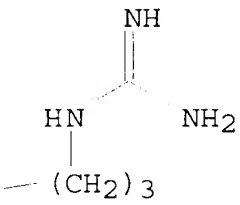
RN 420819-95-0 HCA
CN L-Phenylalanine, L-.alpha.-aspartyl-L-arginyl-4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-tyrosyl-L-isoleucyl-L-histidyl-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

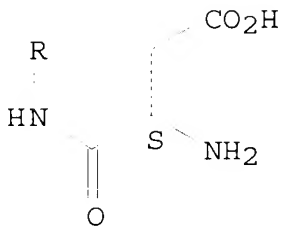
PAGE 1-A



PAGE 1-B



PAGE 2-A

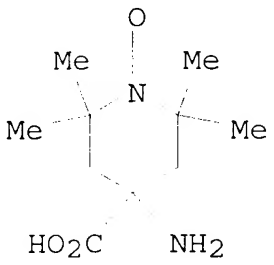


IT **15871-57-5**, TOAC
(**solid phase** peptide **synthesis** and

smooth muscle contraction activity of paramagnetic spin-labeled angiotensin and bradykinin analogs)

RN 15871-57-5 HCA

CN 1-Piperidinyloxy, 4-amino-4-carboxy-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 2, 22

ST angiotensin analog TOAC labeled **solid phase** peptide **synthesis** pharmacol; bradykinin paramagnetic analog spin labeled prepn smooth muscle contraction; EPR mol structure property tetramethylpiperidineoxylaminocarboxylic acid labeled angiotensin bradykinin; muscle contracting structure activity angiotensin bradykinin spin labeled EPR

IT **Solid phase synthesis**
(peptide; **solid phase** peptide **synthesis** and smooth muscle contraction activity of paramagnetic spin-labeled angiotensin and bradykinin analogs)

IT Muscle contraction
(smooth muscle; **solid phase** peptide **synthesis** and smooth muscle contraction activity of paramagnetic spin-labeled angiotensin and bradykinin analogs)

IT Muscle
(smooth; **solid phase** peptide **synthesis** and smooth muscle contraction activity of paramagnetic spin-labeled angiotensin and bradykinin analogs)

IT ESR (electron spin resonance)
(**solid phase** peptide **synthesis** and EPR spectra of paramagnetic spin-labeled angiotensin and bradykinin analogs)

IT Hormones, animal, **preparation**
(**solid phase** peptide **synthesis** and smooth muscle contraction activity of paramagnetic spin-labeled angiotensin and bradykinin analogs)

IT Peptides, **preparation**
(spin labeled; **solid phase** peptide **synthesis** and smooth muscle contraction activity of paramagnetic spin-labeled angiotensin and bradykinin analogs)

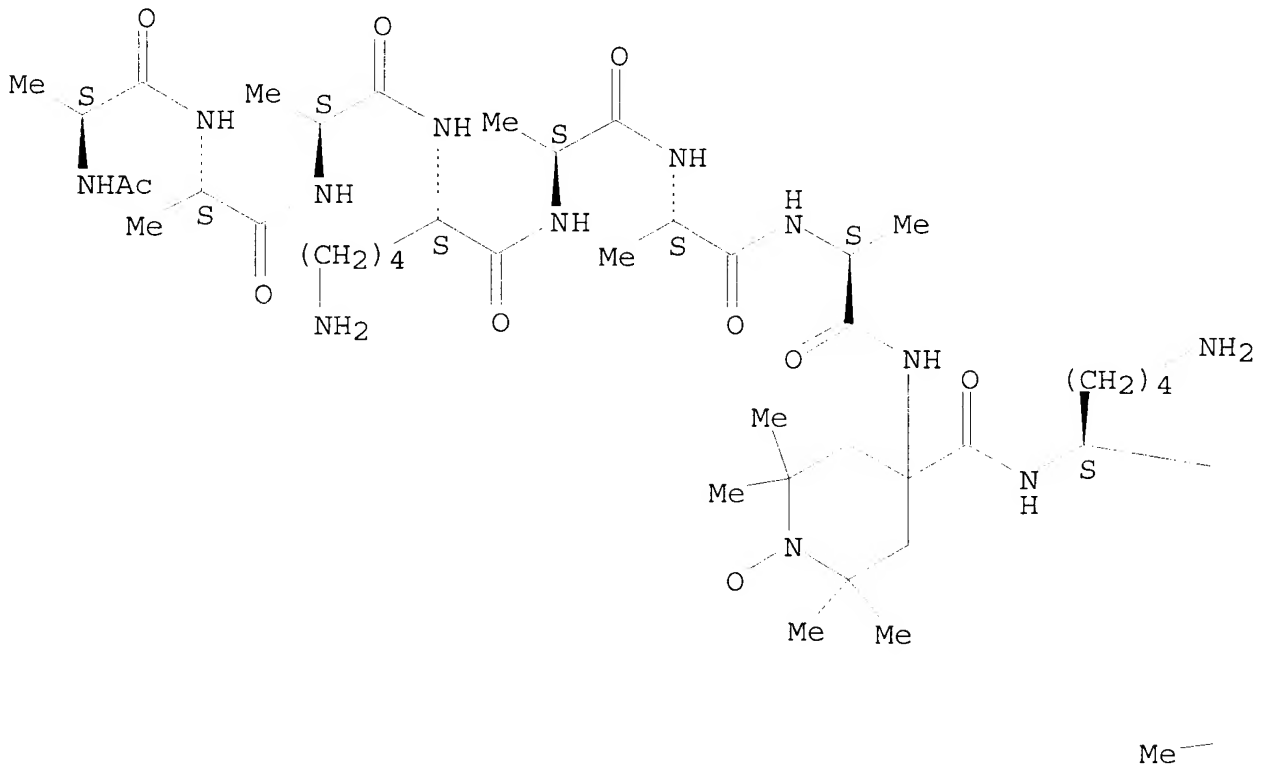
IT 58-82-2DP, Bradykinin, analogs 11128-99-7DP, Angiotensin II, analogs **84606-48-4P 215931-15-0P**
(**solid phase** peptide **synthesis** and smooth muscle contraction activity of paramagnetic spin-labeled

angiotensin and bradykinin analogs)
IT **151842-58-9P 215931-19-4P 420819-95-0P**
(**solid phase** peptide **synthesis** and
smooth muscle contraction activity of paramagnetic spin-labeled
angiotensin and bradykinin analogs)
IT **15871-57-5**, TOAC
(**solid phase** peptide **synthesis** and
smooth muscle contraction activity of paramagnetic spin-labeled
angiotensin and bradykinin analogs)

L44 ANSWER 7 OF 36 HCA COPYRIGHT 2003 ACS
136:232537 **Solid-phase synthesis** of
peptides containing the spin-labeled 2,2,6,6-tetramethylpiperidine-1-oxyl-4-amino-4-carboxylic acid (TOAC). Martin, L.; Ivancich, A.; Vita, C.; Formaggio, F.; Toniolo, C. (Department of Protein Engineering, Commissariat a l'Energie Atomique, Gif-sur-Yvette, 91191, Fr.). Journal of Peptide Research, 58(5), 424-432 (English) 2001. CODEN: JPERFA. ISSN: 1397-002X. Publisher: Munksgaard International Publishers Ltd..
AB 2,2,6,6-Tetramethylpiperidine-1-oxyl-4-amino-4-carboxylic acid (TOAC) is a nitroxide spin-labeled, achiral C.alpha.-tetrasubstituted amino acid recently shown to be not only an effective .beta.-turn and 310/.alpha.-helix promoter in peptides, but also an excellent rigid ESR probe and fluorescence quencher. Here, the authors demonstrate that TOAC can be effectively incorporated into internal positions of peptide sequences using Fmoc chem. and **solid-phase synthesis** in an automated app.
IT **219728-91-3P 219728-92-4P 219728-93-5P**
(**solid-phase synthesis**, CD and EPR
anal. of peptides contg. the spin-labeled amino acid TOAC)
RN 219728-91-3 HCA
CN L-Alaninamide, N-acetyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl-L-alanyl-L-alanyl-L-alanyl-4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-lysyl-4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A


Me
S
NHAc
NH
Me
S
O
Me
S
NH
(CH2)4
NH2
O
NH
Me
S
O
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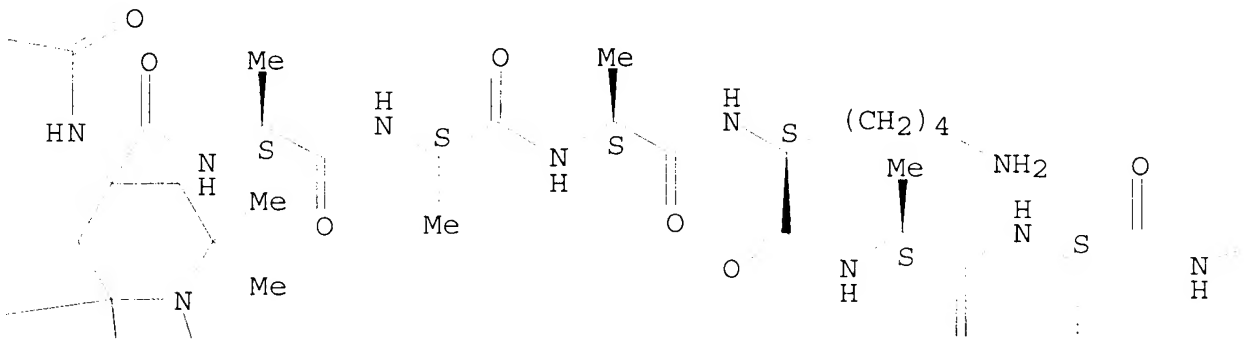
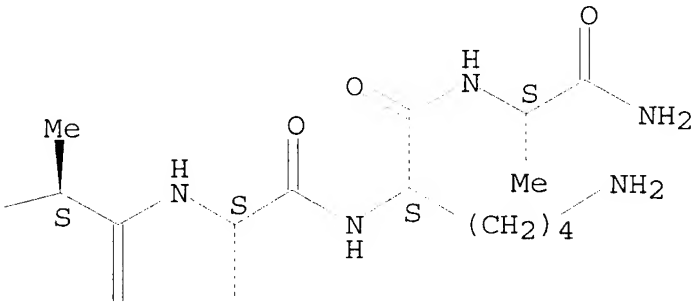
Me
S
O
H
N
S
Me
O
NH
Me
Me
N
O
Me
Me
O
N
H
(CH2)4
NH2
S
Me

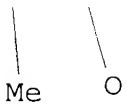
PAGE 1-B



PAGE 1-C



PAGE 2-B



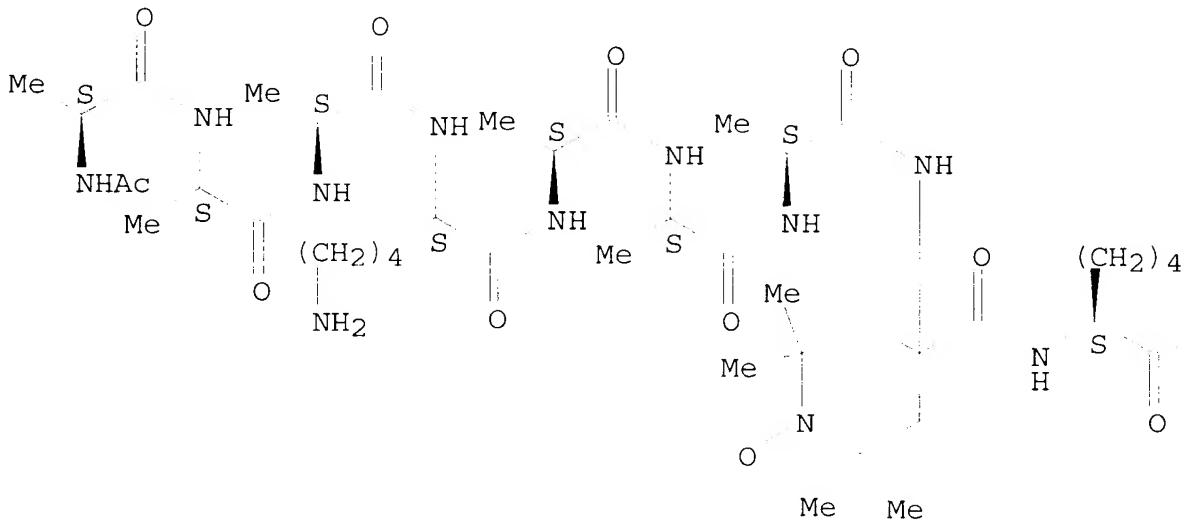
PAGE 2-C

RN 219728-92-4 HCA

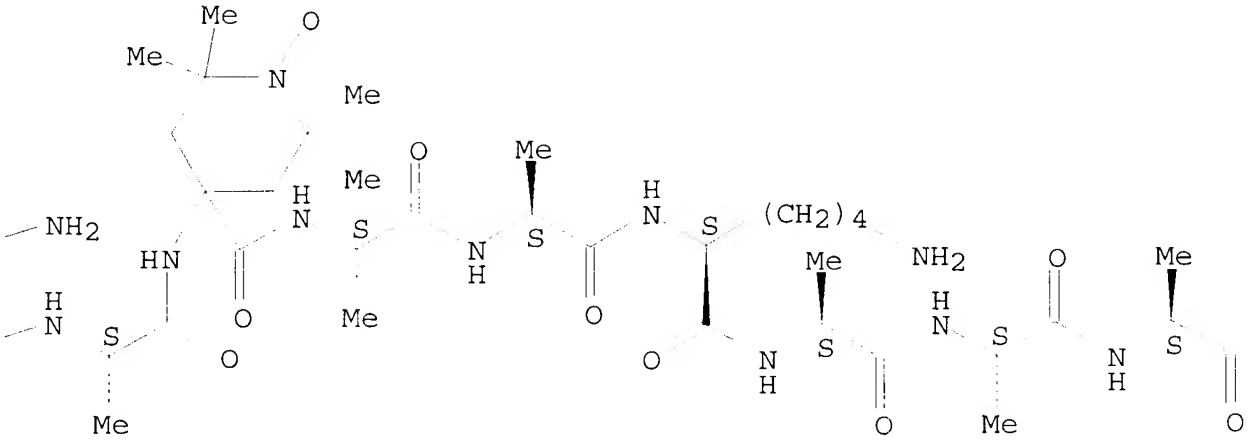
CN L-Alaninamide, N-acetyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl-L-alanyl-L-alanyl-L-alanyl-4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-lysyl-L-alanyl-4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-alanyl-L-alanyl-L-lysyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

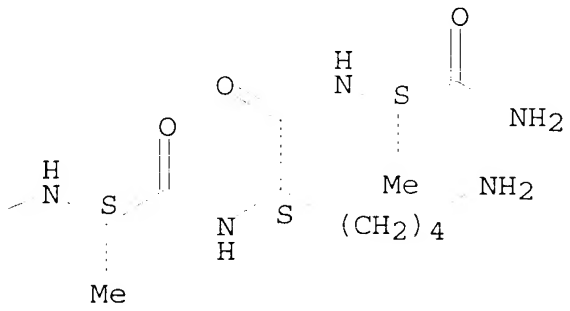
PAGE 1-A



PAGE 1-B



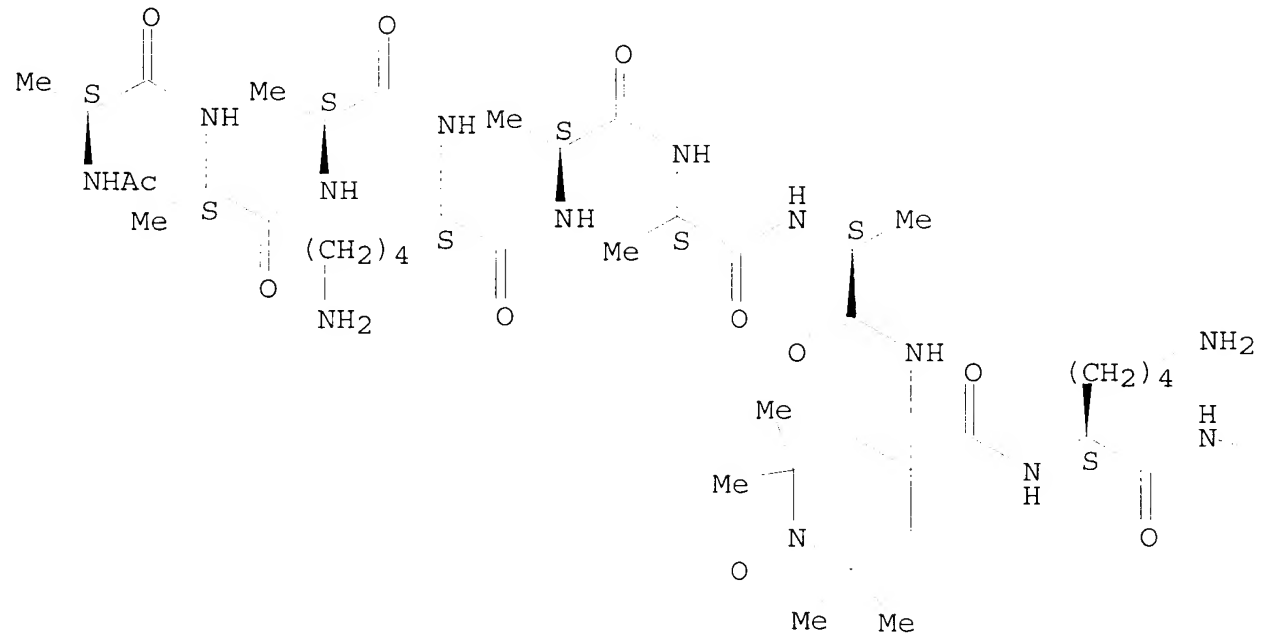
PAGE 1-C



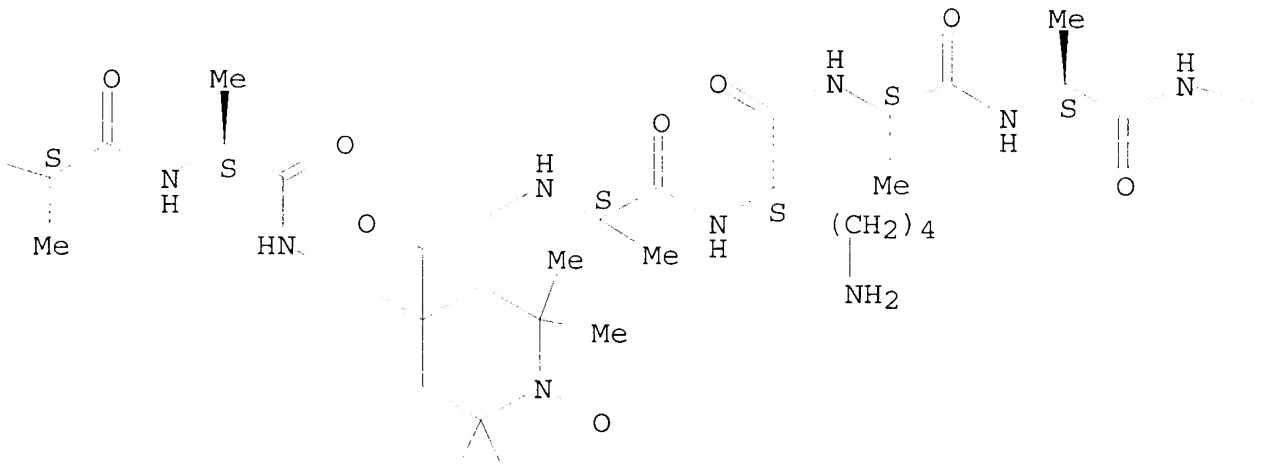
RN 219728-93-5 HCA
CN L-Alaninamide, N-acetyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl-L-alanyl-L-alanyl-L-alanyl-4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-lysyl-L-alanyl-L-alanyl-4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-alanyl-L-lysyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-lysyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

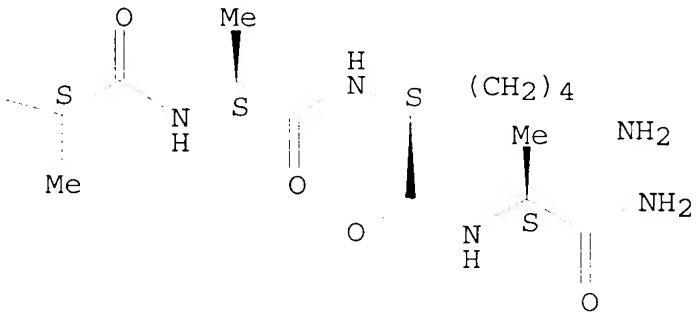
PAGE 1-A



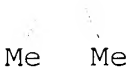
PAGE 1-B



PAGE 1-C



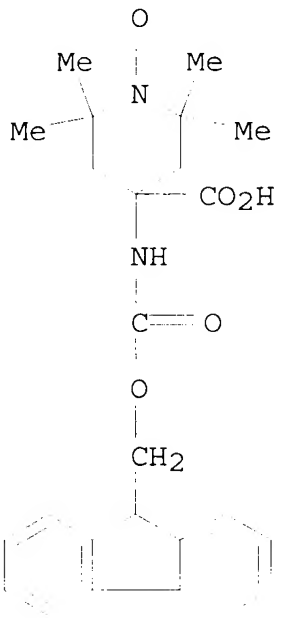
PAGE 2-B



IT **93372-25-9**
(**solid-phase synthesis**, CD and EPR anal. of peptides contg. the spin-labeled amino acid TOAC)

RN 93372-25-9 HCA

CN 1-Piperidinyloxy, 4-carboxy-4-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22
ST peptide spin labeled amino acid TOAC **solid phase synthesis**; conformation spin labeled peptide CD EPR
IT **Solid phase synthesis**
(peptide; **solid-phase synthesis**, CD and EPR anal. of peptides contg. the spin-labeled amino acid TOAC)
IT Conformation
Spin labels
(**solid-phase synthesis**, CD and EPR anal. of peptides contg. the spin-labeled amino acid TOAC)
IT Peptides, **preparation**
(**solid-phase synthesis**, CD and EPR anal. of peptides contg. the spin-labeled amino acid TOAC)
IT **219728-91-3P 219728-92-4P 219728-93-5P**
(**solid-phase synthesis**, CD and EPR anal. of peptides contg. the spin-labeled amino acid TOAC)
IT 35661-39-3 71989-26-9 **93372-25-9**
(**solid-phase synthesis**, CD and EPR anal. of peptides contg. the spin-labeled amino acid TOAC)

L44 ANSWER 8 OF 36 HCA COPYRIGHT 2003 ACS
135:195792 Preparation of vasoactive intestinal peptide analogs as anticancer agents. Burman, Anand C.; Prasad, Sudhanand; Mukherjee, Rama; Singh, Anu T.; Mathur, Archina; Gupta, Neena (Dabur Research Foundation, India). PCT Int. Appl. WO 2001060862 A1 20010823, 34 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB,

GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US20871 20000731. PRIORITY: IN 2000-DE136 20000218.

AB Title peptides H-His-Ser-Asp-X1-Val-X2-Thr-Asp-Asn-Tyr-Thr-Arg-Leu-Arg-Lys-Gln-X3-Ala-Val-Lys-Lys-Tyr-Leu-Asn-Ser-Ile-Leu-Asn-NH2 (X1 = Aib, Deg, Ac5c; X2 = Phe, 4-Cl-D-Phe; R3 = Met, Leu, Dpg; Aib = .alpha.-aminoisobutyrate, Deg = .alpha.,.alpha.-diethylglycine, Ac5c = 1-aminocyclopentanecarboxyl; 4-Cl-D-Phe = 4-chloro-D-phenylalanyl; Dpg = .alpha.,.alpha.-di-n-propylglycine) contg. .alpha.,.alpha.-dialkyl amino acids in a site-specific manner were prepd. For example, H-His-Ser-Asp-Aib-Val-4-Cl-D-Phe-Thr-Asp-Asn-Tyr-Thr-Arg-Leu-Arg-Lys-Gln-Leu-Ala-Val-Lys-Lys-Tyr-Leu-Asn-Ser-Ile-Leu-Asn-NH2 (I) was **prepd**. via **solid-phase synthesis** using Fmoc-Asn(Trt)-resin and Fmoc chem. At 100 pM concn., I demonstrated the following percentage cytotoxicity values against specific tumor cell lines: 16 .+-. 3.3 (PA1, ovary), 16.9 .+-. 4.5 (SW620, colon), 10 .+-. 3.5 (HuTu80, duodenum), 18 .+-. 2.3 (L132, lung), 10.5 .+-. 4.5 (U87MG, glioblastoma), 47 .+-. 8.5 (KB, oral), 20 .+-. 6.5 (MIAPaCa2, pancreas), 16 .+-. 5.5 (A549, non-small cell lung), and 26 .+-. 5.5 (HT29, colon).

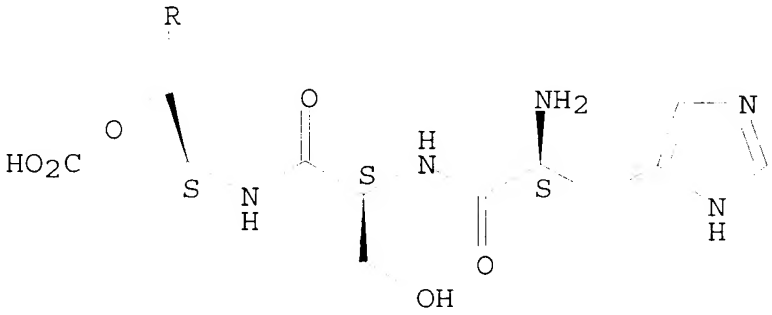
IT **355409-36-8P 355409-39-1P 355409-44-8P**
(prepn. and cytotoxicity activity of antitumor, vasoactive intestinal peptide analogs contg. site-specific dialkylated amino acids)

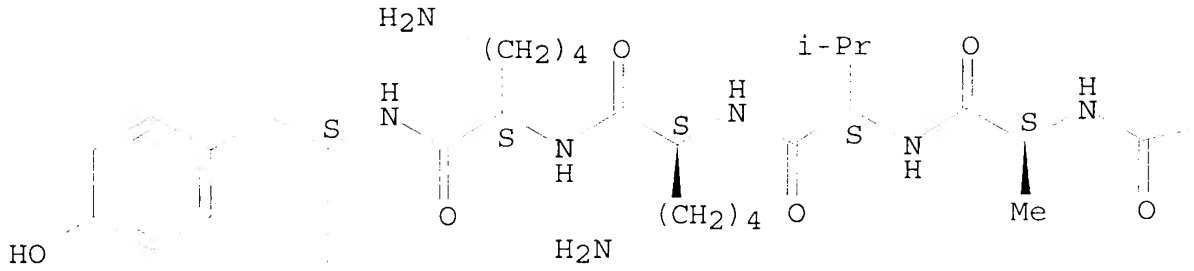
RN 355409-36-8 HCA

CN L-Aspartamide, L-histidyl-L-seryl-L-.alpha.-aspartyl-1-aminocyclopentanecarbonyl-L-valyl-4-chloro-D-phenylalanyl-L-threonyl-L-.alpha.-aspartyl-L-asparaginyl-L-tyrosyl-L-threonyl-L-arginyl-L-leucyl-L-arginyl-L-lysyl-L-glutaminyl-L-leucyl-L-alanyl-L-valyl-L-lysyl-L-lysyl-L-tyrosyl-L-leucyl-L-asparaginyl-L-seryl-L-isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)

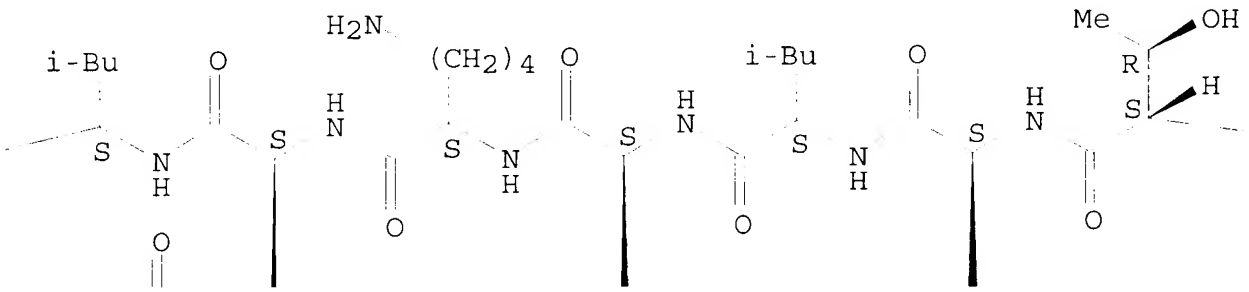
Absolute stereochemistry.

PAGE 1-A

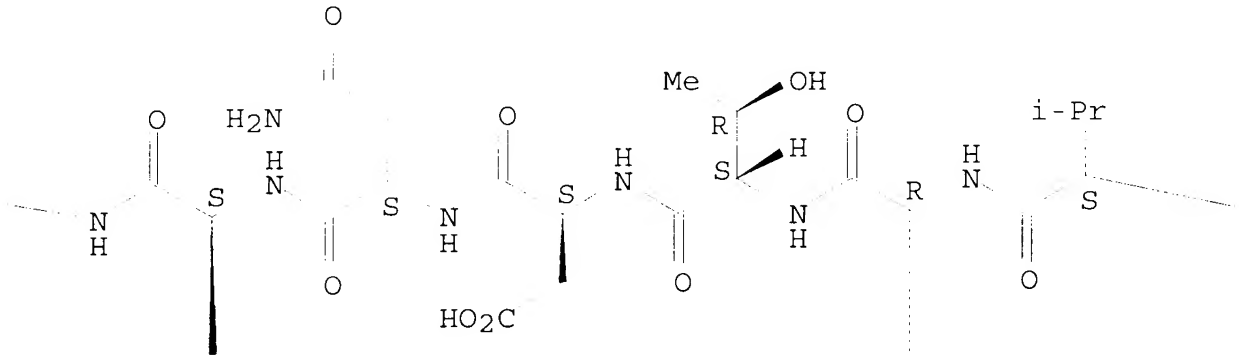




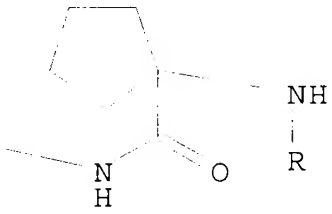
PAGE 1-B



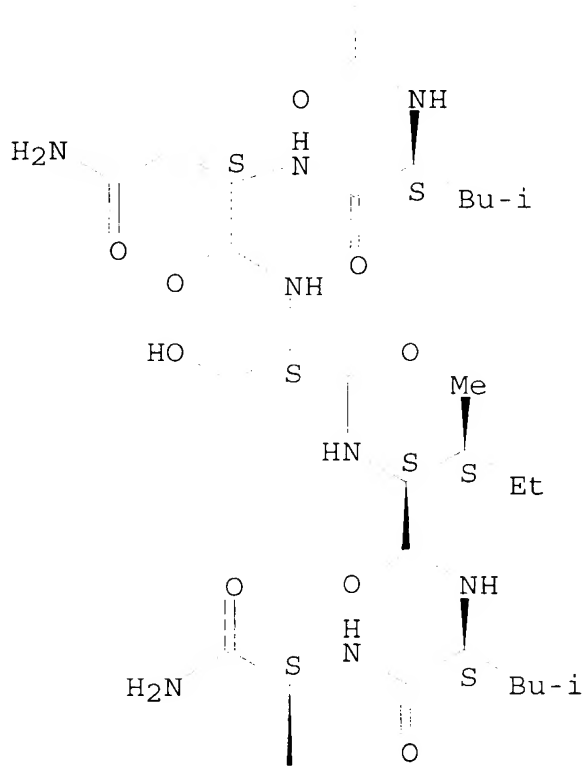
PAGE 1-C



PAGE 1-D



PAGE 2-A



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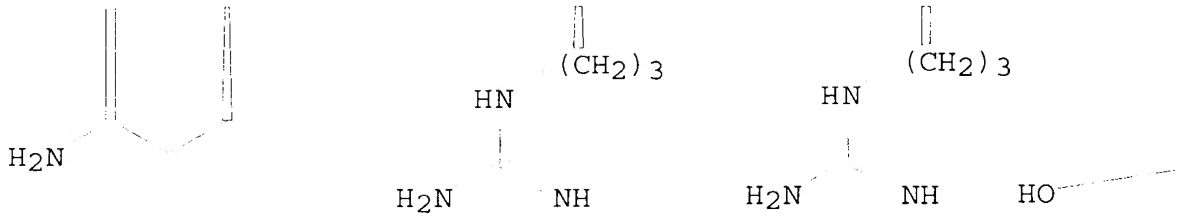
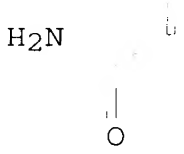


PAGE 2-C

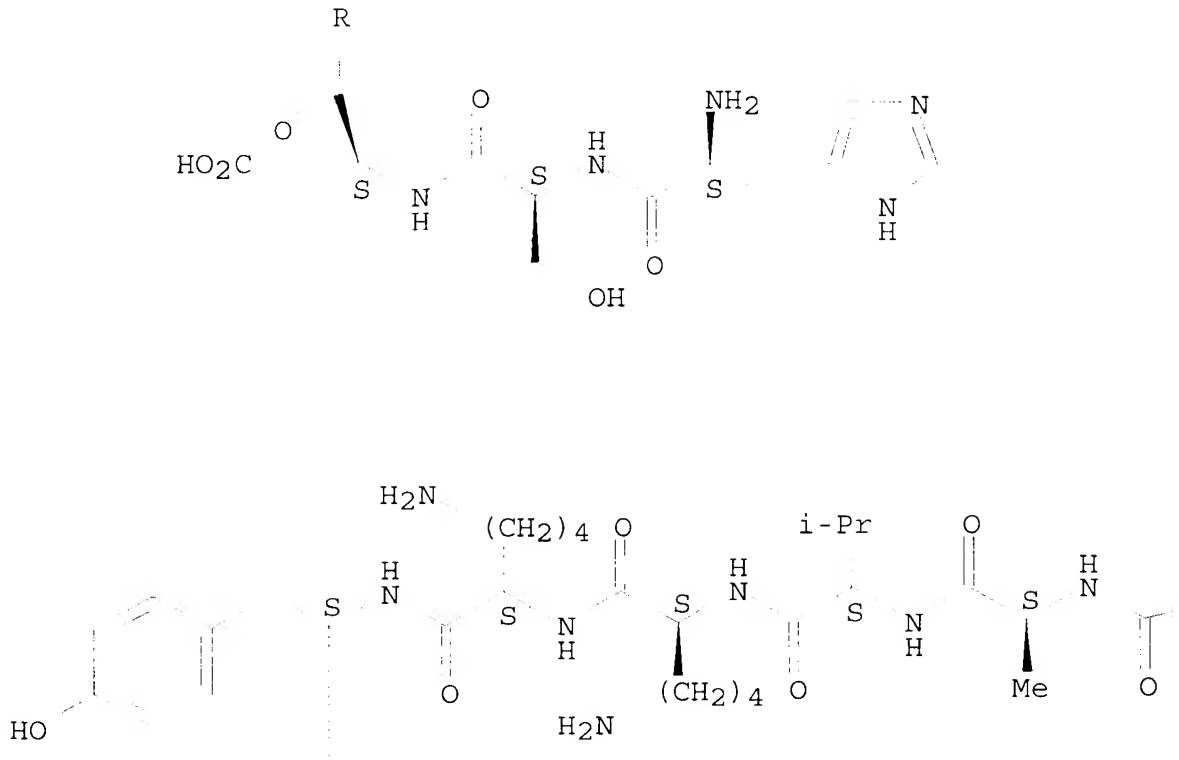
PAGE 3-A



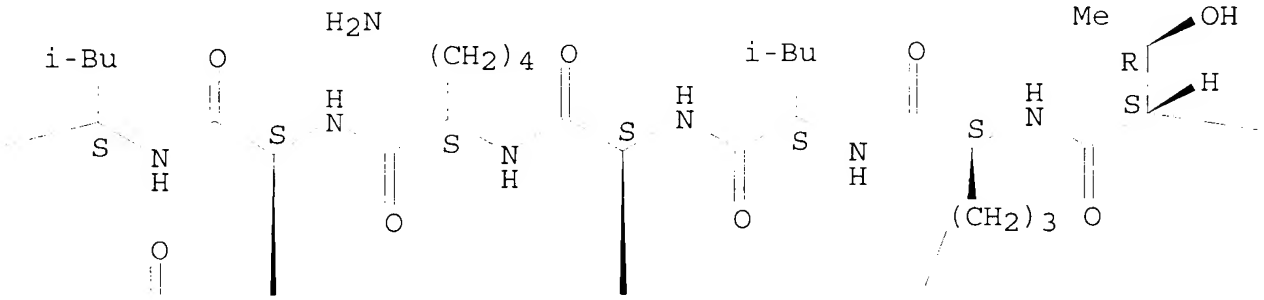
RN 355409-39-1 HCA
CN L-Aspartamide, L-histidyl-L-seryl-L-.alpha.-aspartyl-1-aminocyclopentanecarbonyl-L-valyl-L-phenylalanyl-L-threonyl-L-.alpha.-aspartyl-L-asparaginyl-L-tyrosyl-L-threonyl-L-arginyl-L-leucyl-L-arginyl-L-lysyl-L-glutaminyl-L-leucyl-L-alanyl-L-valyl-L-lysyl-L-lysyl-L-tyrosyl-L-leucyl-L-asparaginyl-L-seryl-L-isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

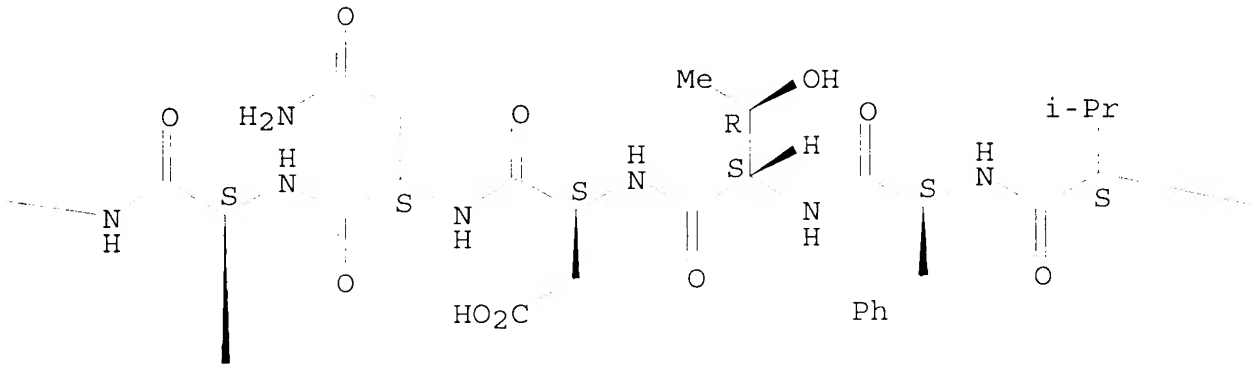
PAGE 1-A



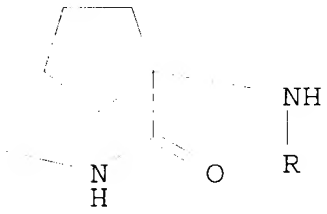
PAGE 1-B



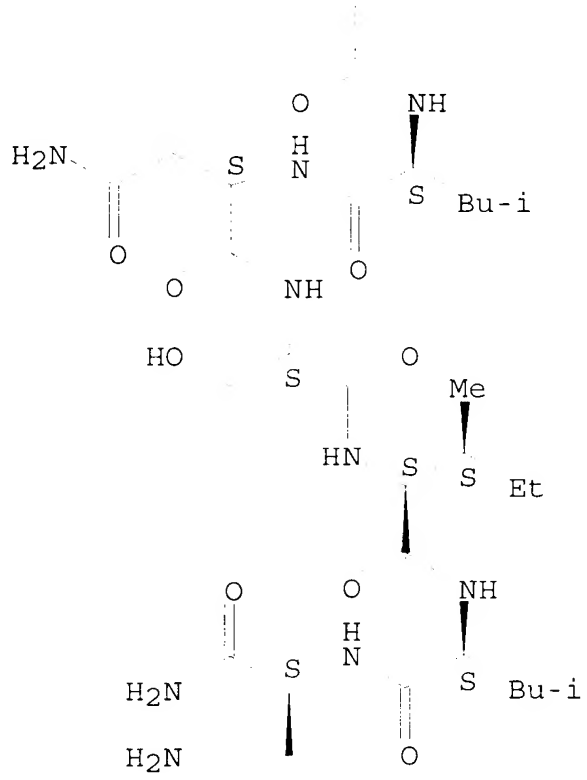
PAGE 1-C



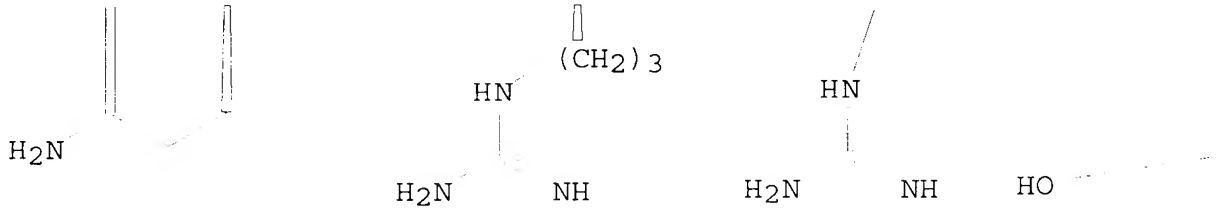
PAGE 1-D



PAGE 2-A



PAGE 2-B



PAGE 2-C

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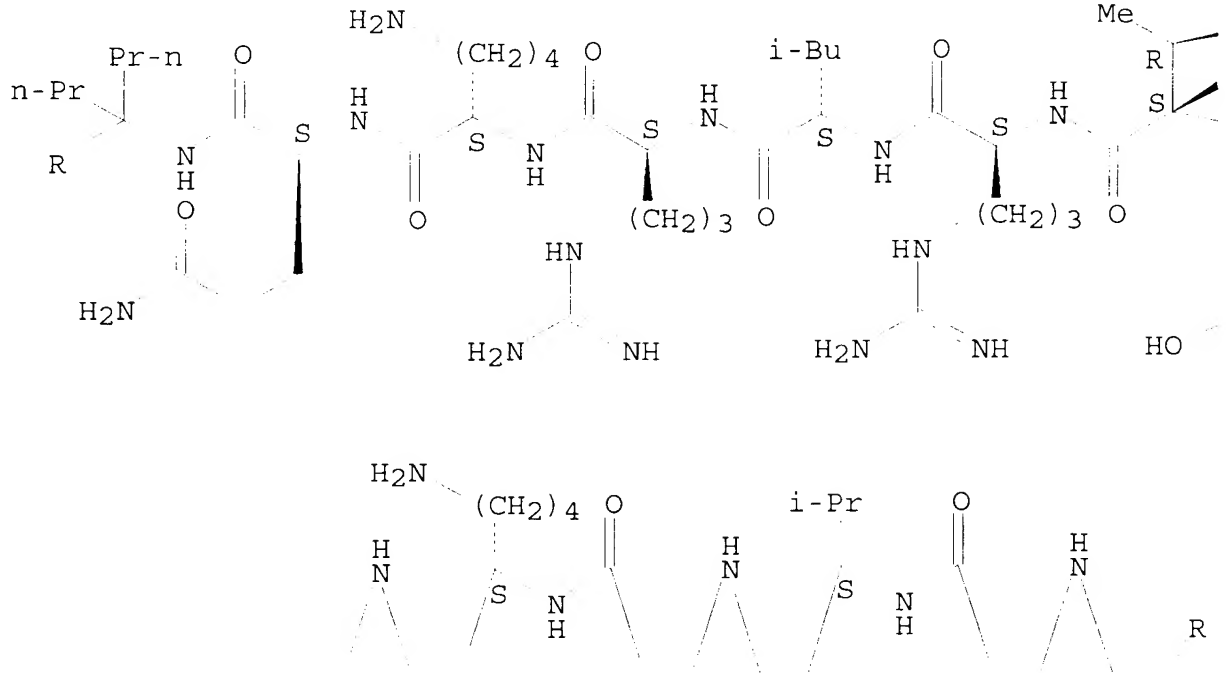
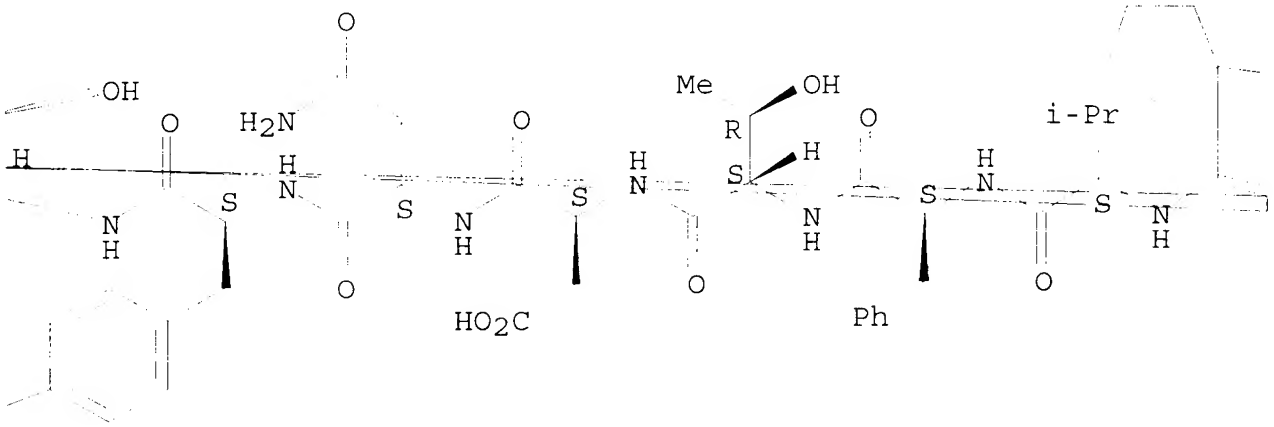
RN 355409-44-8 HCA
CN L-Aspartamide, L-histidyl-L-seryl-L-.alpha.-aspartyl-1-aminocyclopentanecarbonyl-L-valyl-L-phenylalanyl-L-threonyl-L-.alpha.-aspartyl-L-asparaginyl-L-tyrosyl-L-threonyl-L-arginyl-L-leucyl-L-arginyl-L-lysyl-L-glutaminyl-2-propylnorvalyl-L-alanyl-L-valyl-L-lysyl-L-lysyl-L-tyrosyl-L-leucyl-L-asparaginyl-L-seryl-L-isoleucyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

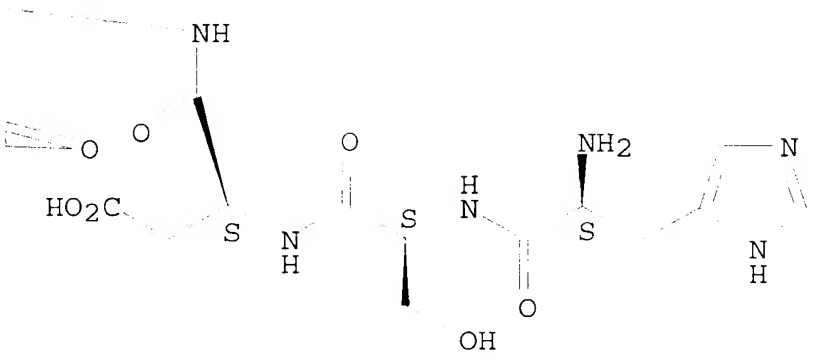
PAGE 1-A



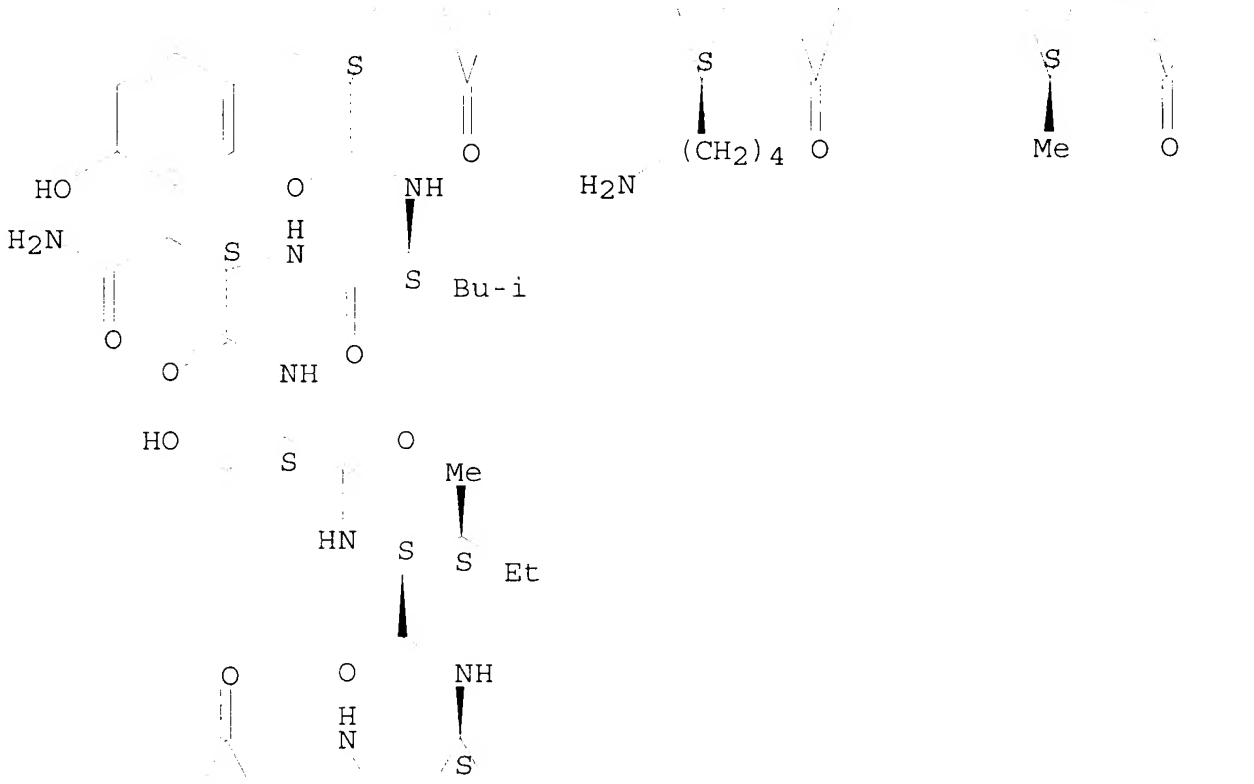
PAGE 1-B



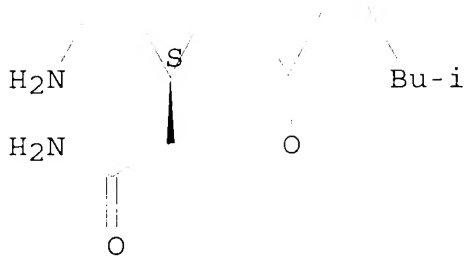
PAGE 1-C



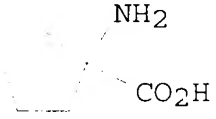
PAGE 2-A



PAGE 3-A



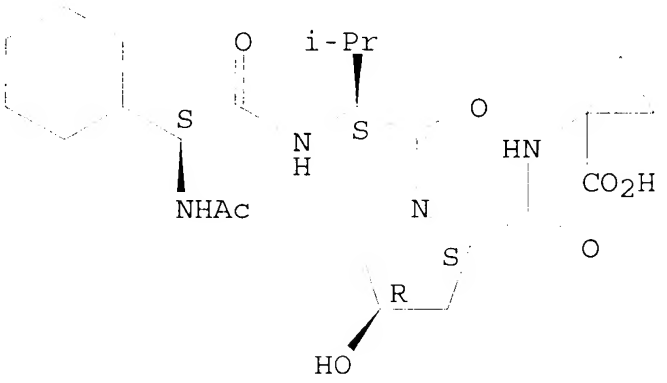
IT **52-52-8P**
(prepn. of dialkylated amino acids)
RN 52-52-8 HCA
CN Cyclopentanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IC C07K014-575; A61K038-22; A61P035-00
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1
IT 40077-57-4DP, Vasoactive intestinal octacosapeptide (swine), .alpha.,.alpha.-dialkyl amino acid-contg. analogs 355409-34-6P 355409-35-7P **355409-36-8P** 355409-37-9P 355409-38-0P **355409-39-1P** 355409-40-4P 355409-41-5P 355409-42-6P 355409-43-7P **355409-44-8P**
(prepn. and cytotoxicity activity of antitumor, vasoactive intestinal peptide analogs contg. site-specific dialkylated amino acids)
IT **52-52-8P**
(prepn. of dialkylated amino acids)

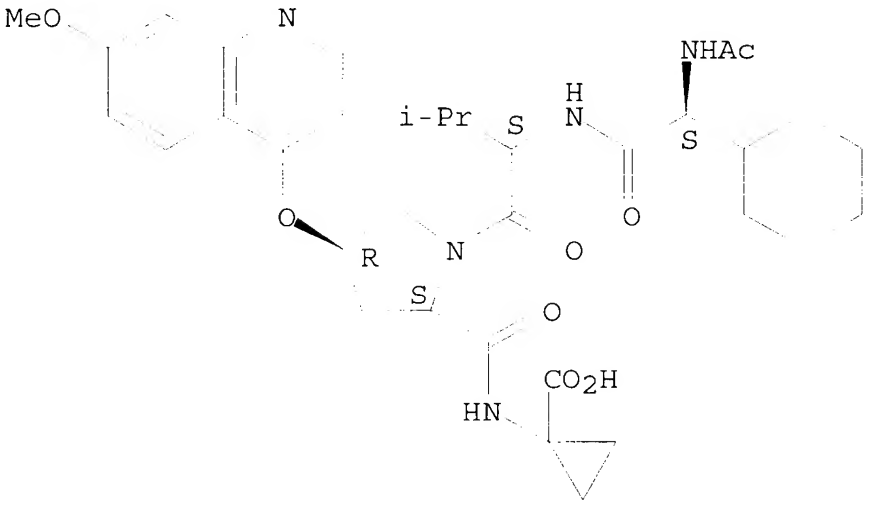
L44 ANSWER 9 OF 36 HCA COPYRIGHT 2003 ACS
135:195782 **Solid-Phase Synthesis** of Peptidomimetic Inhibitors for the Hepatitis C Virus NS3 Protease. Poupart, Marc-Andre; Cameron, Dale R.; Chabot, Catherine; Ghiro, Elise; Goudreau, Nathalie; Goulet, Sylvie; Poirier, Martin; Tsantrizos, Youla S. (Department of Chemistry, Boehringer Ingelheim (Canada) Ltd., QC, H7S 2G5, Can.). Journal of Organic Chemistry, 66(14), 4743-4751 (English) 2001. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.
AB The NS3 serine protease enzyme of the hepatitis C virus (HCV) is essential for viral replication. Short peptides mimicking the N-terminal substrate cleavage products of the NS3 protease are known to act as weak inhibitors of the enzyme and have been used as templates for the design of peptidomimetic inhibitors. Automated **solid-phase synthesis** of a small library of compds. based on such a peptidomimetic scaffold has led to the identification of potent and highly selective inhibitors of the NS3 protease enzyme.
IT **357292-85-4P 357293-16-4P**
(**solid-phase synthesis** of peptidomimetic inhibitors for the hepatitis C virus NS3 protease)
RN 357292-85-4 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-hydroxy-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 357293-16-4 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(7-methoxy-4-quinolinyl)oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



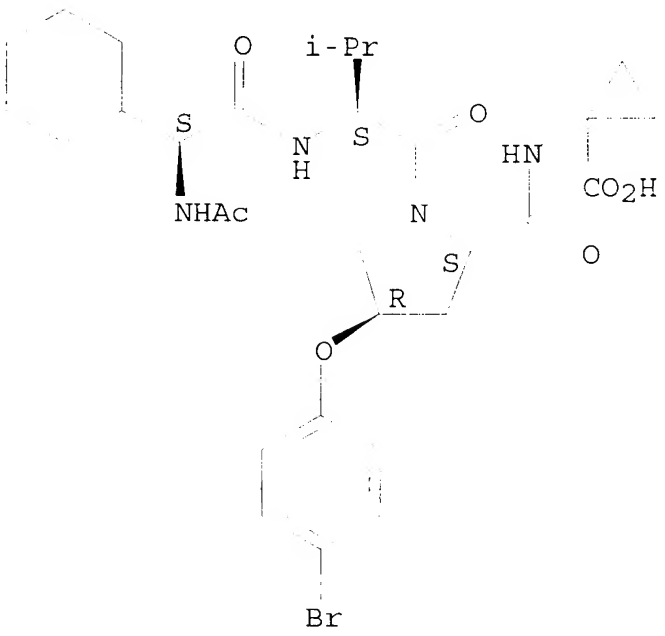
IT **357292-86-5P 357292-87-6P 357292-88-7P**
357292-89-8P 357292-90-1P 357292-91-2P
357292-92-3P 357292-93-4P 357292-94-5P
357292-95-6P 357292-96-7P 357292-97-8P
357292-98-9P 357292-99-0P 357293-00-6P
357293-01-7P 357293-02-8P 357293-03-9P
357293-04-0P 357293-05-1P 357293-06-2P
357293-07-3P 357293-08-4P 357293-09-5P
357293-10-8P 357293-11-9P 357293-12-0P
357293-13-1P 357293-14-2P 357293-15-3P
357293-17-5P
(solid-phase synthesis of

peptidomimetic inhibitors for the hepatitis C virus NS3 protease)

RN 357292-86-5 HCA

CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(4-bromophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

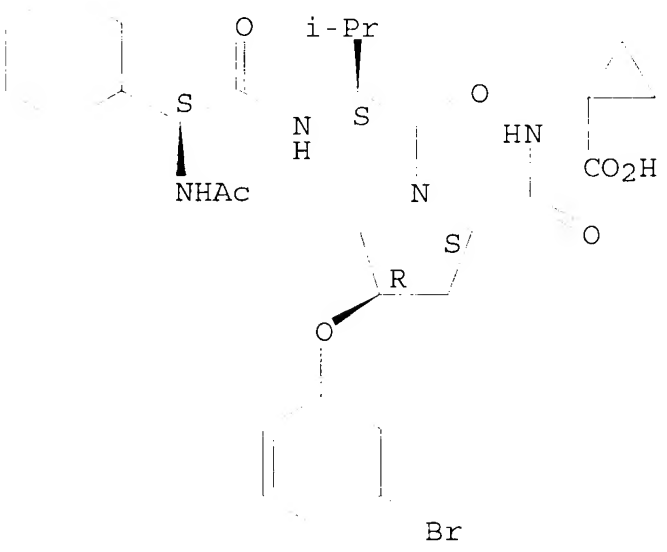
Absolute stereochemistry.



RN 357292-87-6 HCA

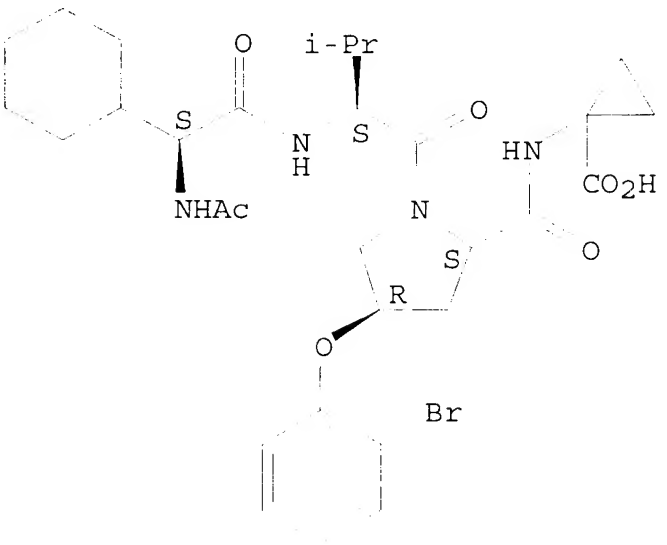
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(3-bromophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



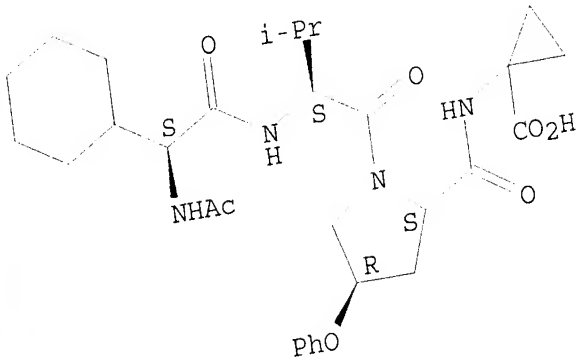
RN 357292-88-7 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(2-bromophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



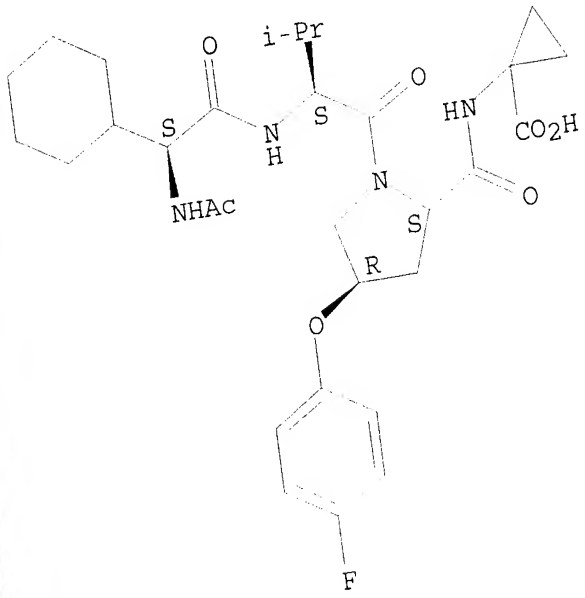
RN 357292-89-8 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-phenoxy-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



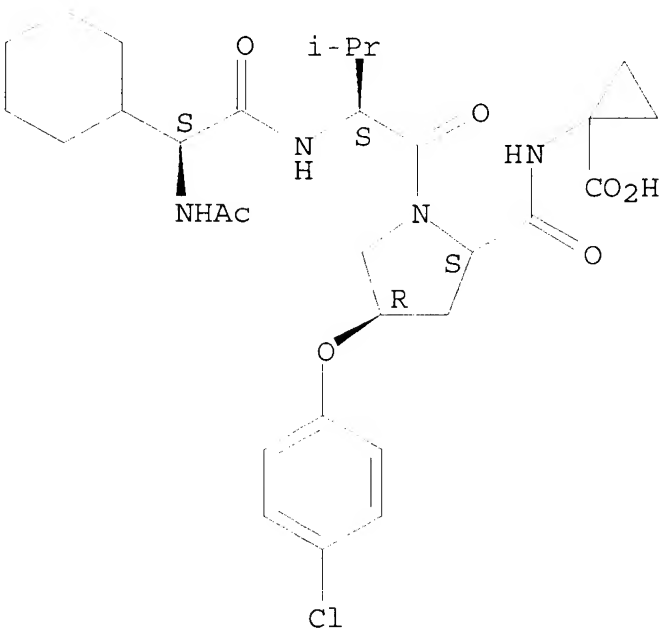
RN 357292-90-1 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(4-fluorophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



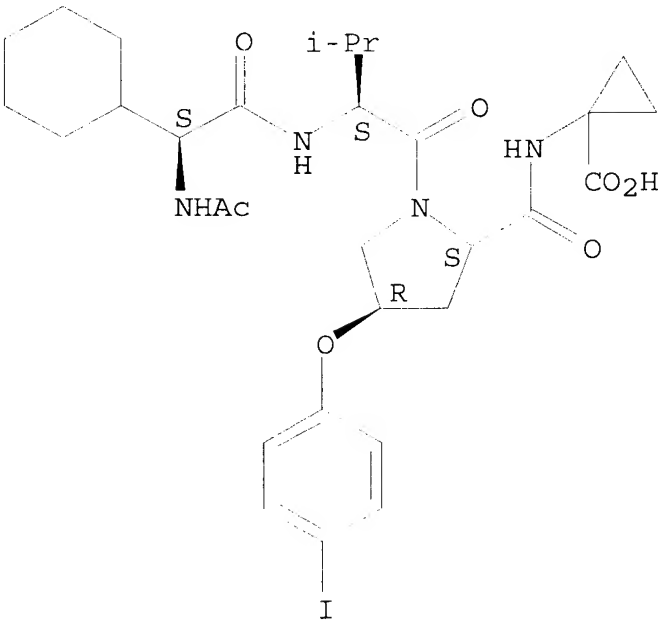
RN 357292-91-2 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(4-chlorophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 357292-92-3 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(4-iodophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

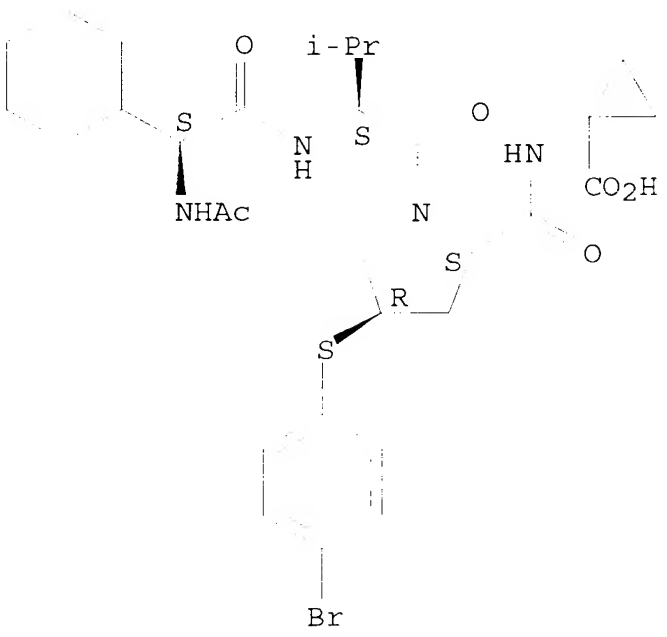
Absolute stereochemistry.



RN 357292-93-4 HCA

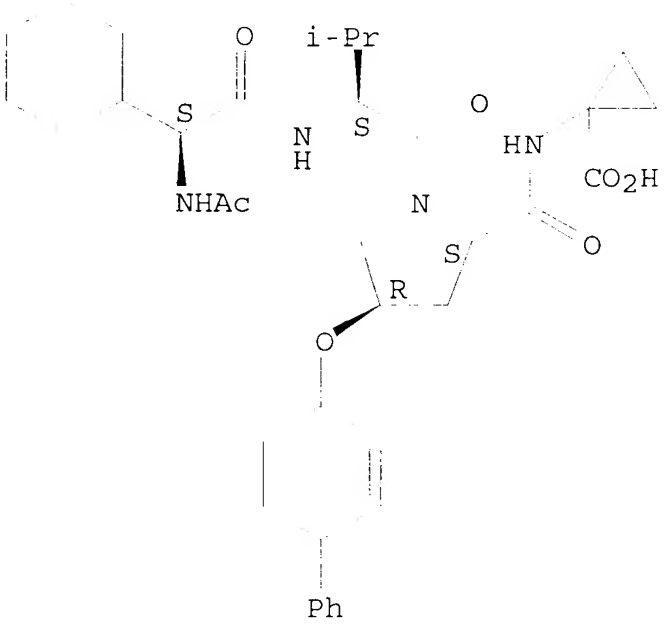
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(4-bromophenyl)thio]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 357292-94-5 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-([1,1'-biphenyl]-4-yloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

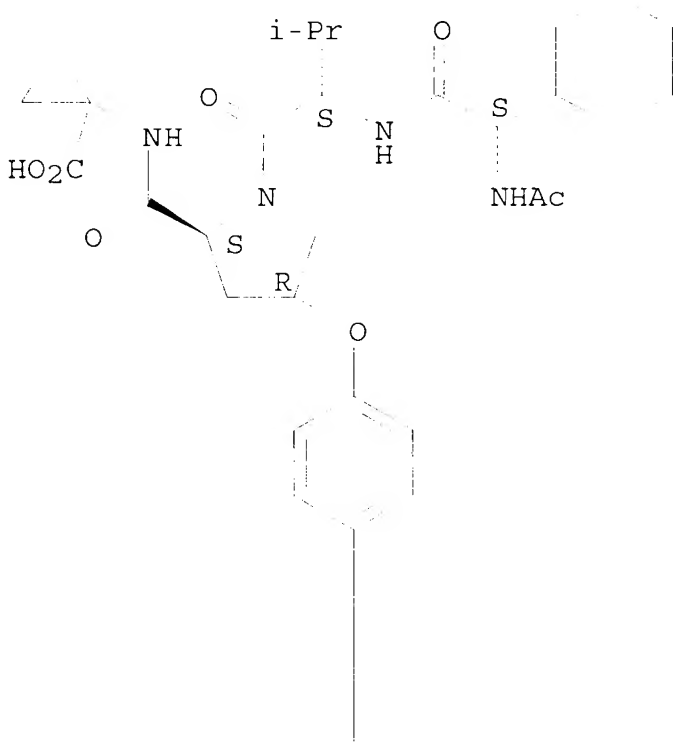
Absolute stereochemistry.



RN 357292-95-6 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(4'-methoxy[1,1'-biphenyl]-4-yl)oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

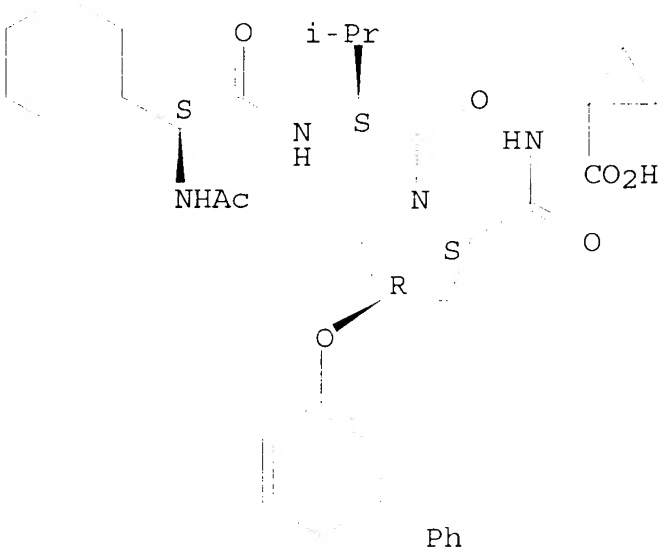
PAGE 1-A



PAGE 2-A

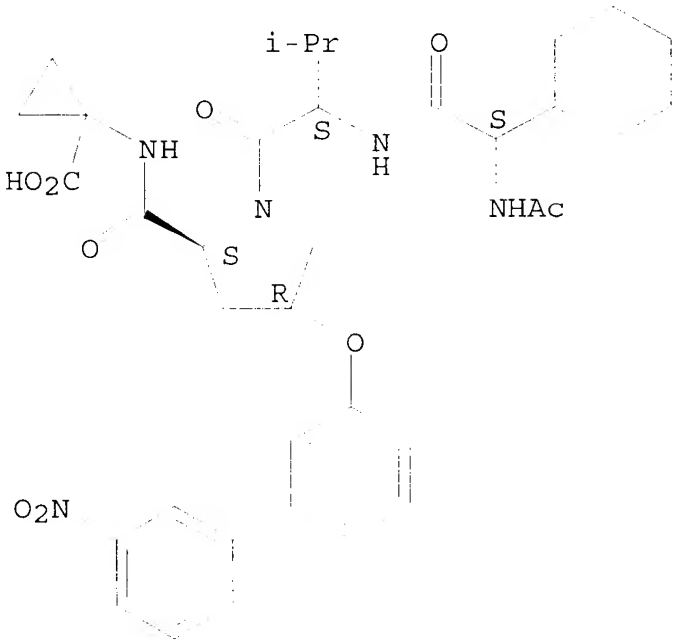
RN 357292-96-7 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-([1,1'-biphenyl]-3-yloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 357292-97-8 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(3'-nitro[1,1'-biphenyl]-3-yl)oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

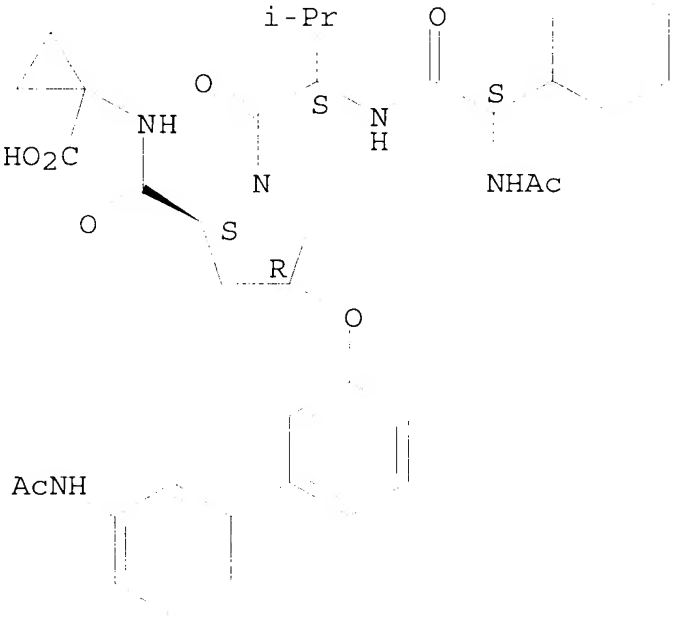
Absolute stereochemistry.



RN 357292-98-9 HCA

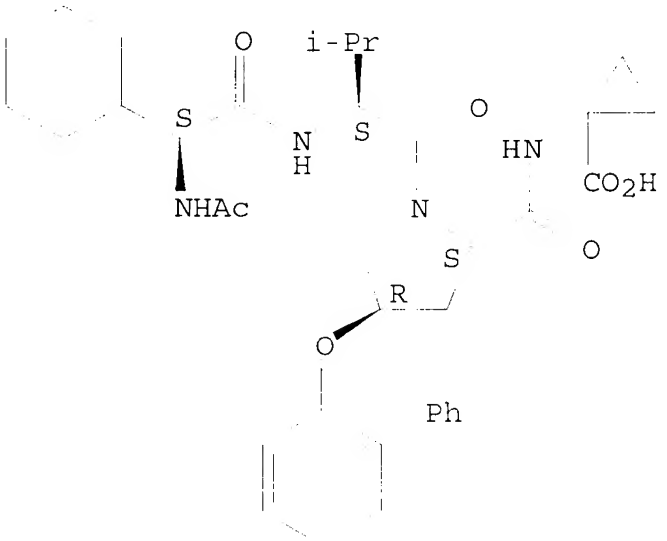
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[[3'-(acetylamino)[1,1'-biphenyl]-3-yl]oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



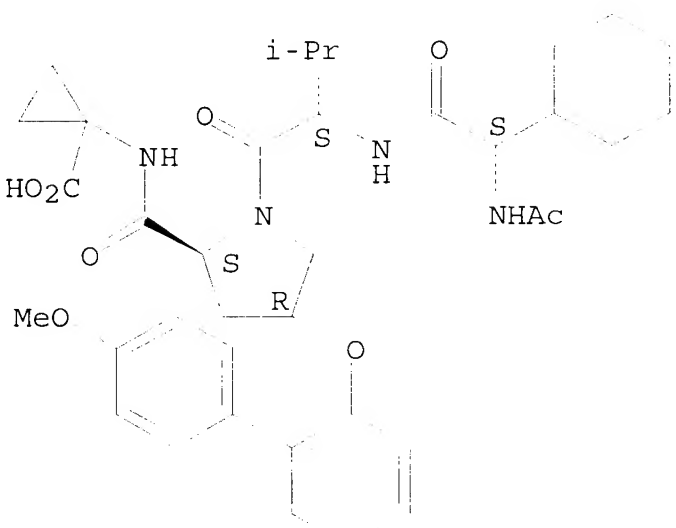
RN 357292-99-0 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-([1,1'-biphenyl]-2-yloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



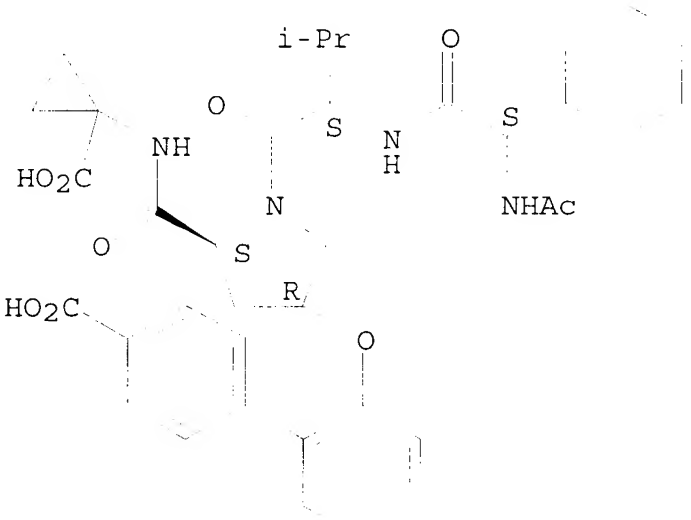
RN 357293-00-6 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(4'-methoxy[1,1'-biphenyl]-2-yl)oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



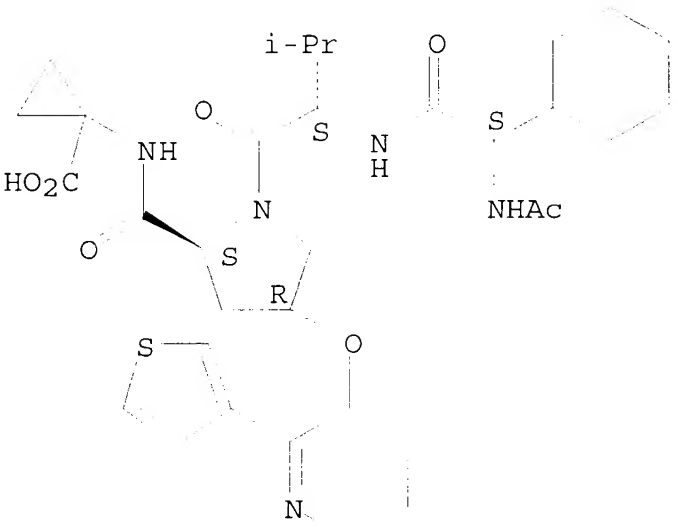
RN 357293-01-7 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(4'-carboxy[1,1'-biphenyl]-2-yl)oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



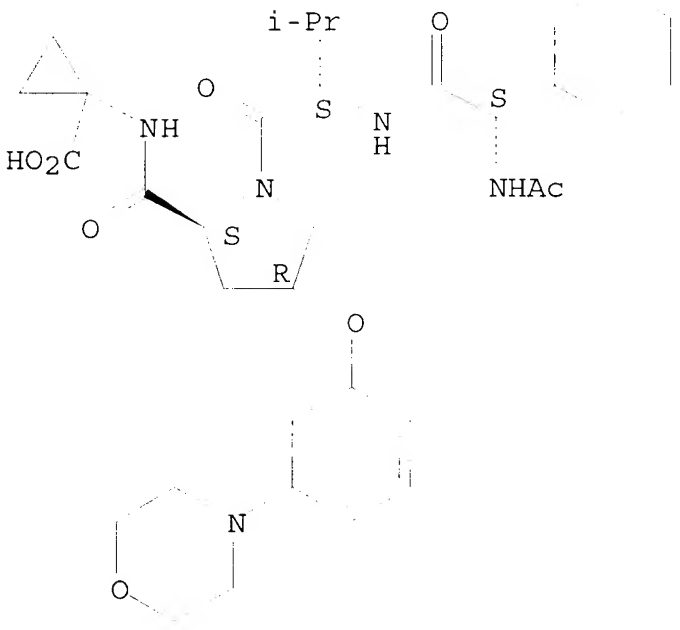
RN 357293-02-8 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[[2-(3-thienyl)-3-pyridinyl]oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



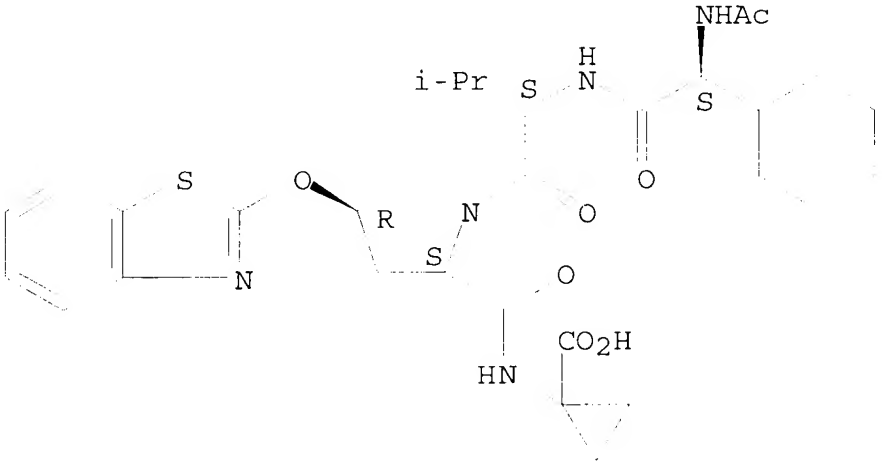
RN 357293-03-9 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[3-(4-morpholinyl)phenoxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 357293-04-0 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(2-benzothiazolyloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

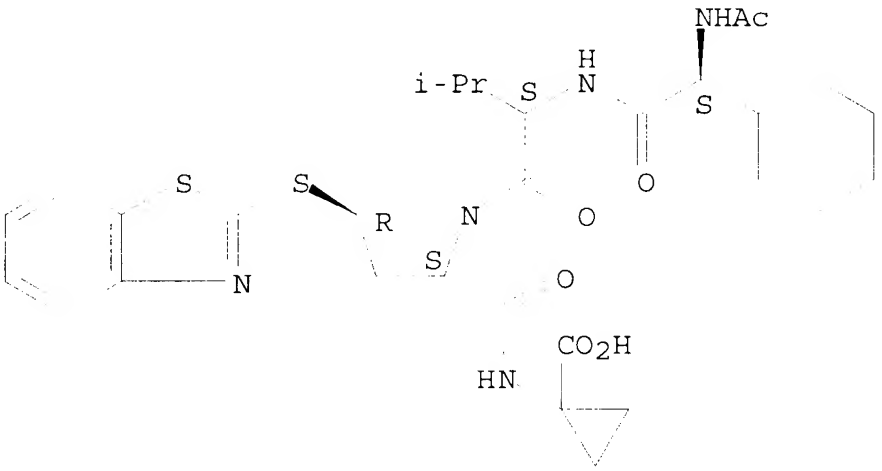
Absolute stereochemistry.



RN 357293-05-1 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(2-benzothiazolylthio)-L-prolyl-1-amino- (9CI) (CA

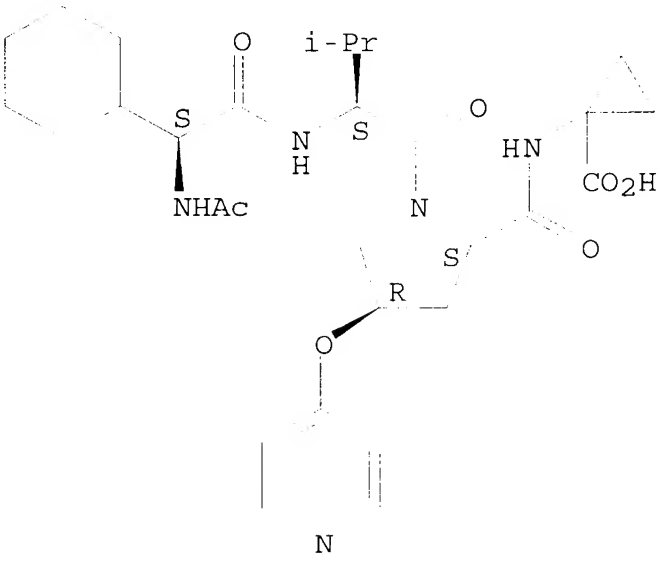
INDEX NAME)

Absolute stereochemistry.



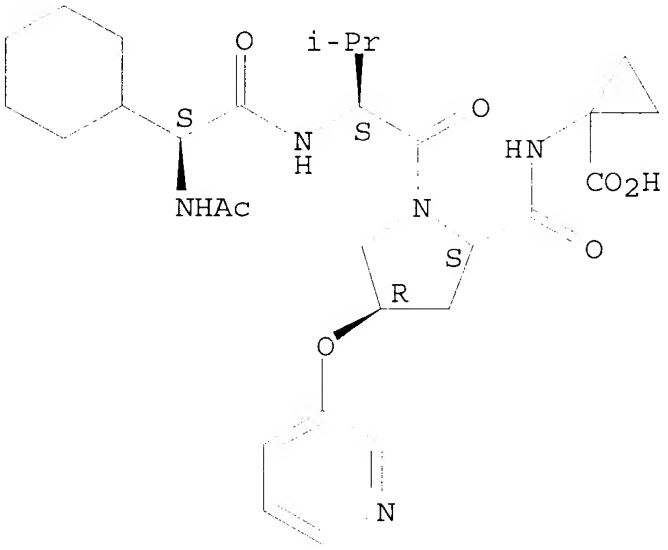
RN 357293-06-2 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(4-pyridinyloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



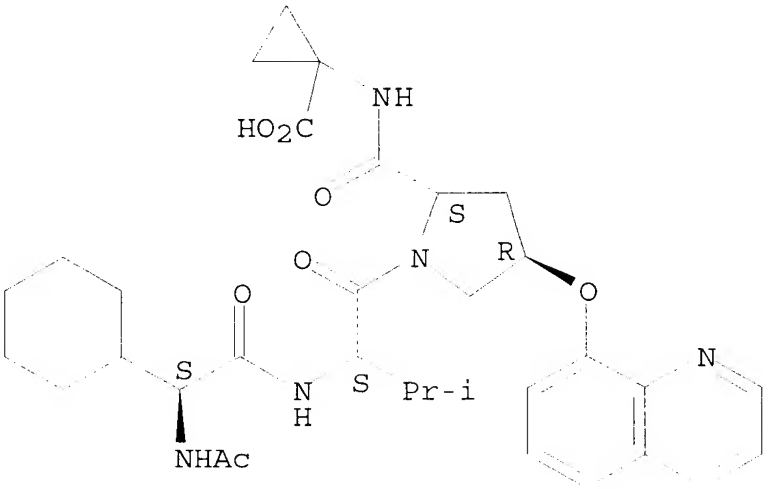
RN 357293-07-3 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(3-pyridinyloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



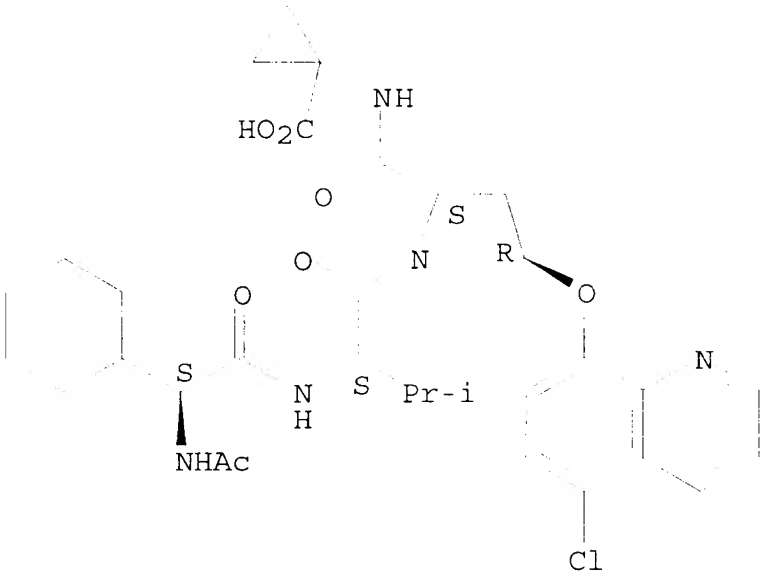
RN 357293-08-4 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(8-quinolinyloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



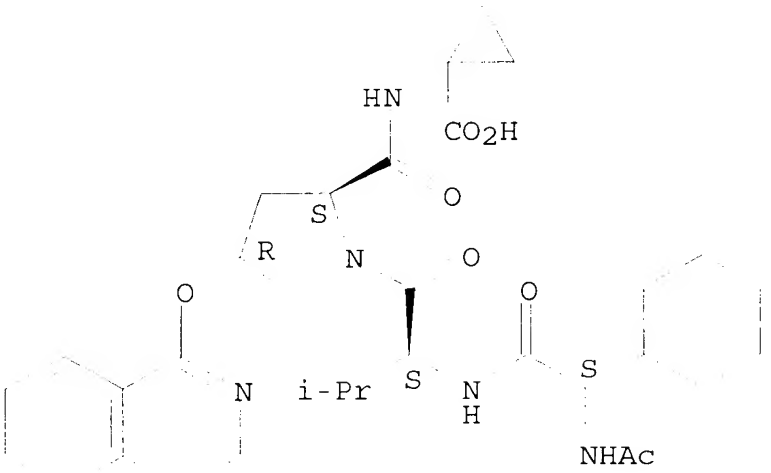
RN 357293-09-5 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(5-chloro-8-quinolinyl)oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



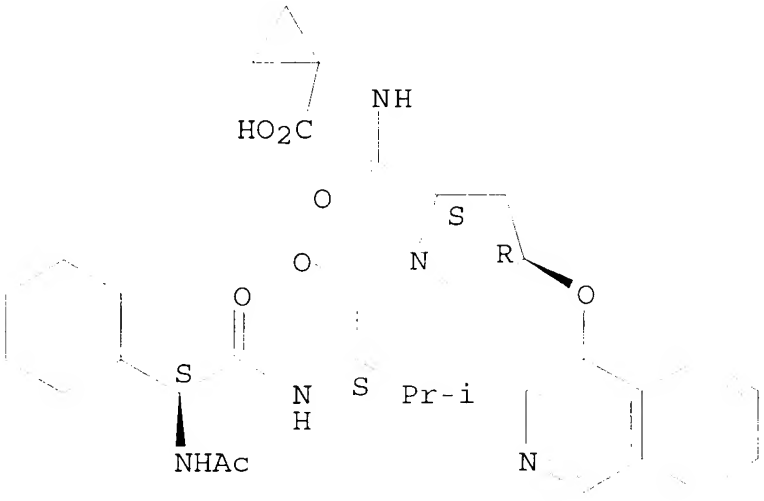
RN 357293-10-8 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(1-isoquinolinyloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



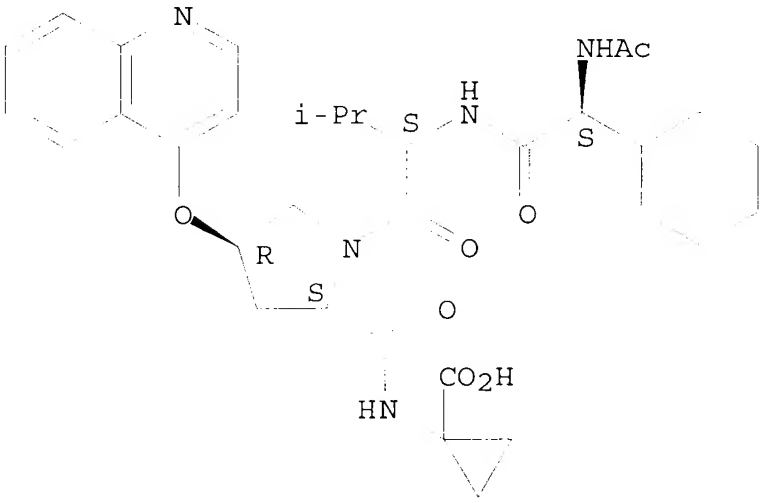
RN 357293-11-9 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(4-isoquinolinyloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



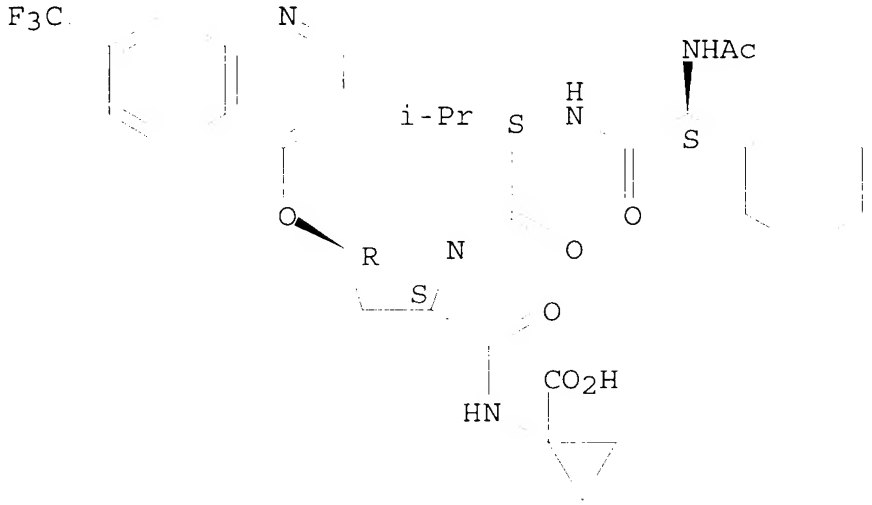
RN 357293-12-0 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(4-quinolinyloxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



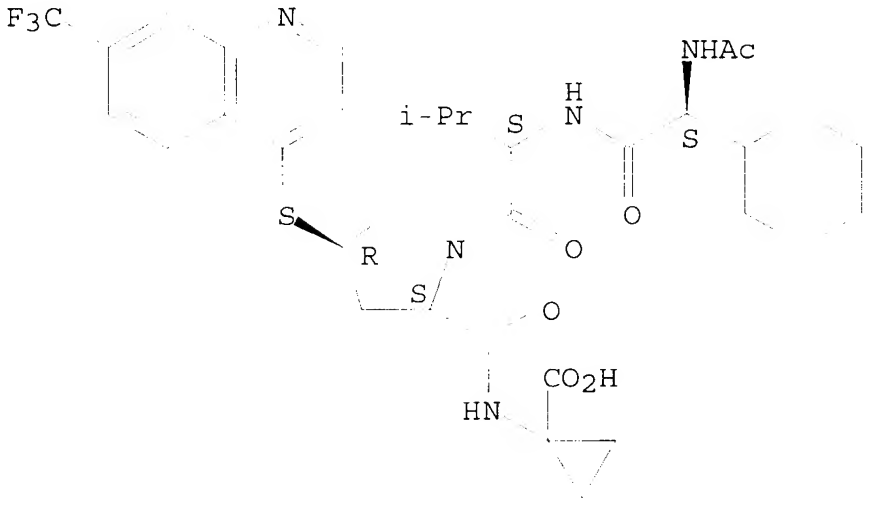
RN 357293-13-1 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[[7-(trifluoromethyl)-4-quinolinyl]oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



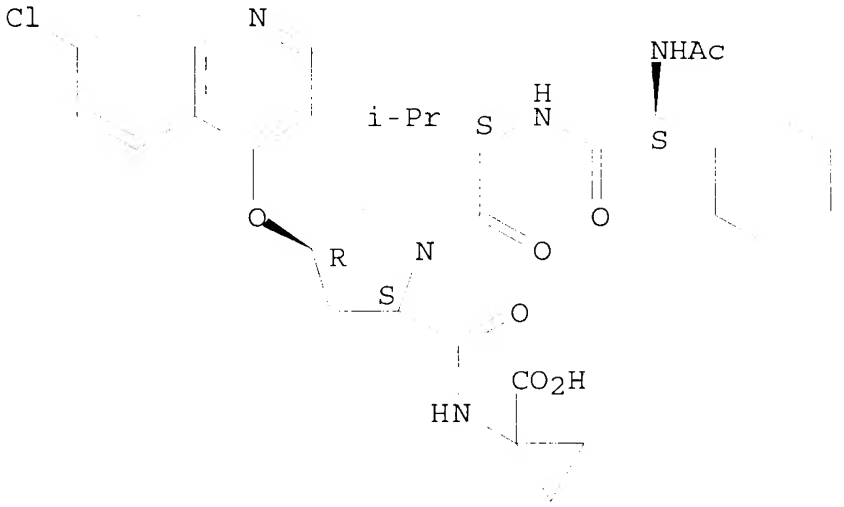
RN 357293-14-2 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[[7-(trifluoromethyl)-4-quinolinyl]thio]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



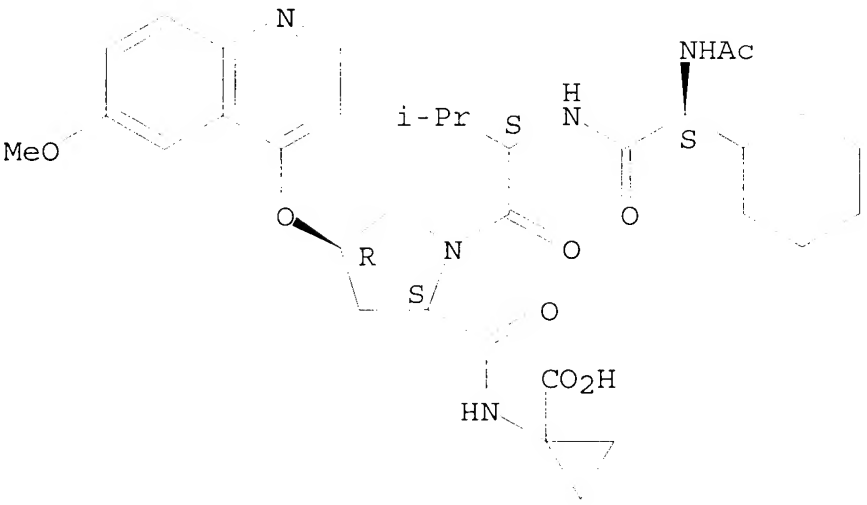
RN 357293-15-3 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(7-chloro-4-quinolinyl)oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 357293-17-5 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-[(6-methoxy-4-quinolinyl)oxy]-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

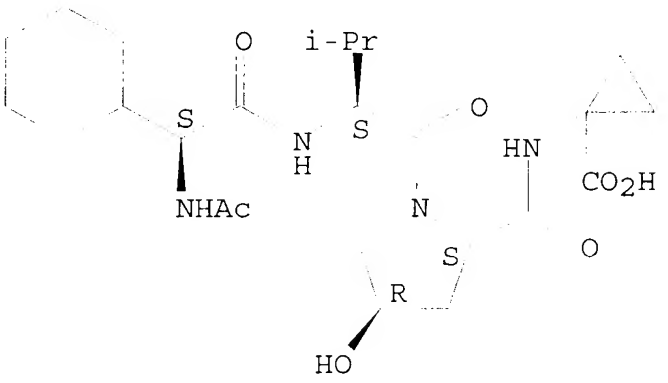
Absolute stereochemistry.



IT **357292-85-4DP, polymer-bound**
357292-86-5DP, polymer-bound
357292-87-6DP, polymer-bound
357292-88-7DP, polymer-bound
(solid-phase synthesis of peptidomimetic inhibitors for the hepatitis C virus NS3 protease)
RN 357292-85-4 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-

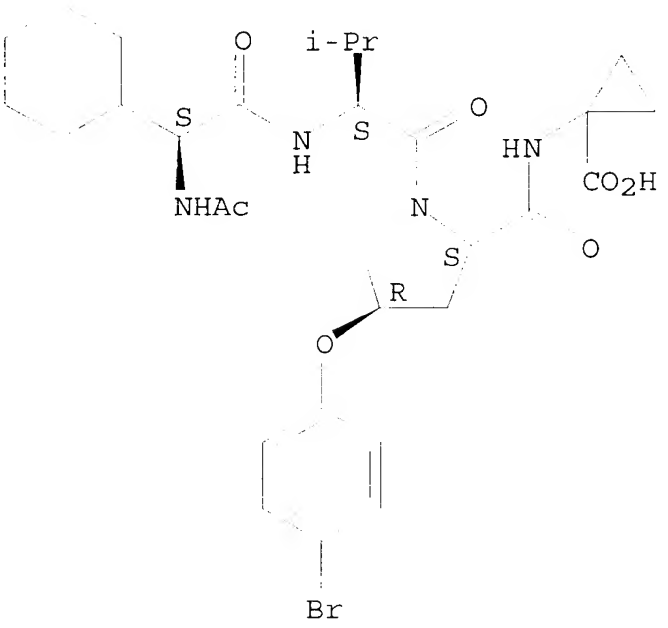
valyl-(4R)-4-hydroxy-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



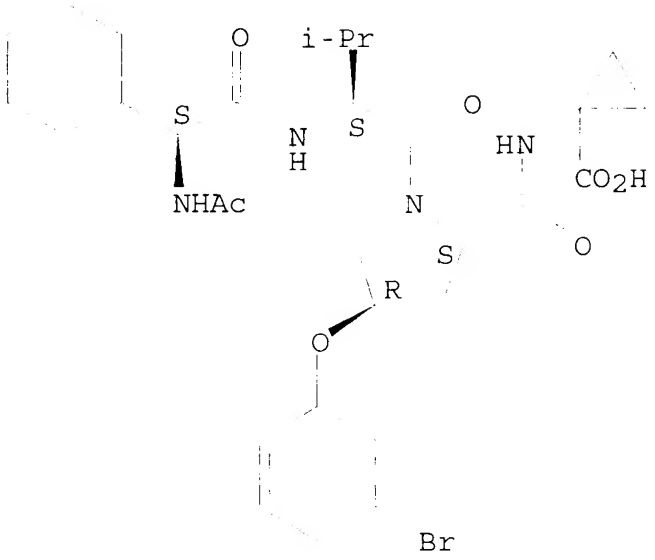
RN 357292-86-5 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(4-bromophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



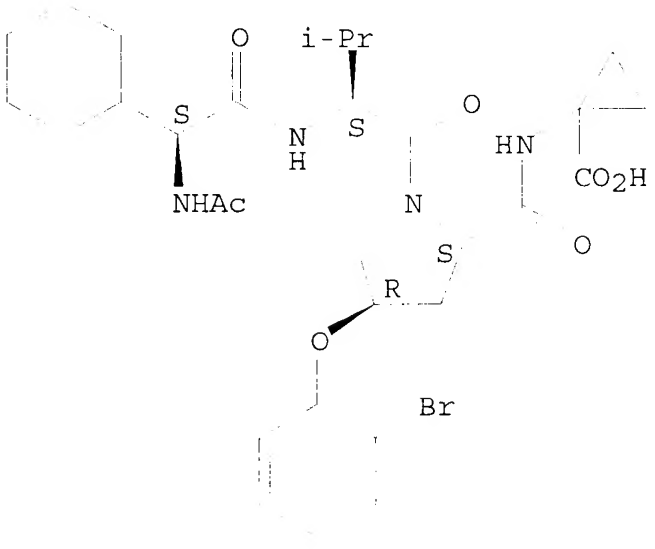
RN 357292-87-6 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(3-bromophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 357292-88-7 HCA
CN Cyclopropanecarboxylic acid, (2S)-N-acetyl-2-cyclohexylglycyl-L-valyl-(4R)-4-(2-bromophenoxy)-L-prolyl-1-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7, 15
ST **solid phase synthesis** peptidomimetic

inhibitor NS3 protease; peptidomimetic prepn inhibitor hepatitis C virus NS3 protease; peptide library inhibitor hepatitis C virus NS3 protease

IT **Solid phase synthesis**
(peptide; **solid-phase synthesis** of peptidomimetic inhibitors for the hepatitis C virus NS3 protease)

IT Hepatitis C virus
Peptide library
Peptidomimetics
(**solid-phase synthesis** of peptidomimetic inhibitors for the hepatitis C virus NS3 protease)

IT **357292-85-4P 357293-16-4P**
(**solid-phase synthesis** of peptidomimetic inhibitors for the hepatitis C virus NS3 protease)

IT **357292-86-5P 357292-87-6P 357292-88-7P**
357292-89-8P 357292-90-1P 357292-91-2P
357292-92-3P 357292-93-4P 357292-94-5P
357292-95-6P 357292-96-7P 357292-97-8P
357292-98-9P 357292-99-0P 357293-00-6P
357293-01-7P 357293-02-8P 357293-03-9P
357293-04-0P 357293-05-1P 357293-06-2P
357293-07-3P 357293-08-4P 357293-09-5P
357293-10-8P 357293-11-9P 357293-12-0P
357293-13-1P 357293-14-2P 357293-15-3P
357293-17-5P
(**solid-phase synthesis** of peptidomimetic inhibitors for the hepatitis C virus NS3 protease)

IT 149885-80-3P, ns3 protease
(**solid-phase synthesis** of peptidomimetic inhibitors for the hepatitis C virus NS3 protease)

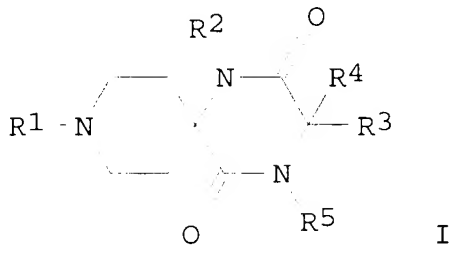
IT **357292-85-4DP, polymer-bound**
357292-86-5DP, polymer-bound
357292-87-6DP, polymer-bound
357292-88-7DP, polymer-bound
(**solid-phase synthesis** of peptidomimetic inhibitors for the hepatitis C virus NS3 protease)

L44 ANSWER 10 OF 36 HCA COPYRIGHT 2003 ACS

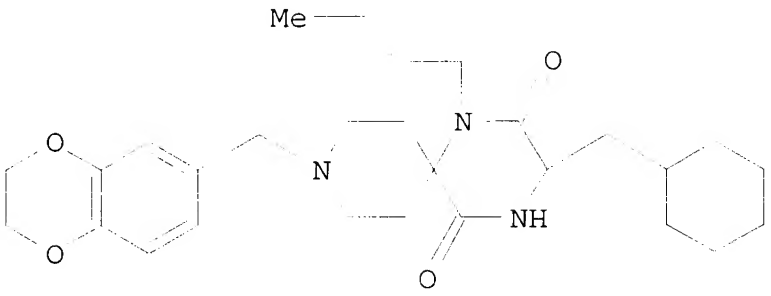
135:46203 Preparation and effect of triazaspiro[5.5]undecane derivatives as active ingredients in remedy for inflammatory diseases. Habashita, Hiromu; Hamano, Shinichi; Shibayam, Shiro; Takaoka, Yoshikazu (Ono Pharmaceutical Co., Ltd., Japan). PCT Int. Appl. WO 2001040227 A1 20010607, 1149 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2000-JP8517 20001201. PRIORITY: JP 1999-344967 19991203; JP

2000-18673 20000127; JP 2000-27968 20000304; JP 2000-147882 20000519.

GI



I



II

AB Title compds. [I; R1 = H, aryl, arylalkyloxycarbonyl, alkenyloxycarbonyl, heterocyclylalkyl, alkyl, alkenyl, alkynyl; R2 = alkyl, alkynyl; R3 = H; R4 = alkyl; R5 = H, alkyl], stereoisomers, quaternary ammonium salts thereof, N-oxides thereof and nontoxic salts thereof, are prepd. via solid phase synthesis using divinylbenzene-polystyrene or divinylbenzene-Rink resin. Title compds. I, having controlling effects of chemokines/chemokine receptors, are useful in preventing and/or treating various inflammatory diseases, asthma, atopic dermatitis, urticaria, allergic diseases, nephritis, nephropathy, hepatitis, arthritis, rheumatoid arthritis, etc. Thus, the title compd. II.cntdot.HCl was prepd. and biol. tested.

IC C07D471-10; A61K031-499; A61K031-5377; A61P029-00; A61P011-06; A61P017-00; A61P017-04; A61P037-08; A61P013-12; A61P001-16; A61P019-02; A61P029-00; A61P017-06; A61P027-16; A61P027-14; A61P009-10; A61P001-04

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

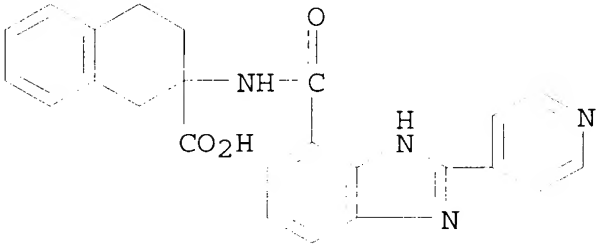
L44 ANSWER 11 OF 36 HCA COPYRIGHT 2003 ACS
134:42443 Preparation and use of benzimidazole derivatives for treatment of illness.. Ritzeler, Olaf; Stilz, Hans Ulrich; Neises, Bernhard; Bock, William Jerome, Jr.; Walser, Armin; Flynn, Gary A. (Aventis Pharma Deutschland G.m.b.H., Germany). Ger. Offen. DE 19928424 A1 20001228, 36 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1999-19928424 19990623.
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

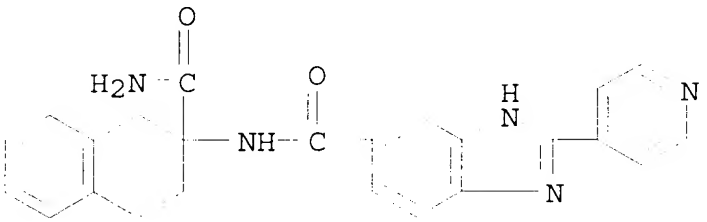
AB Title compds., e.g. (I), were prepd. (no data) for use in treating diseases which feature an intensified activity by transcription factor NF.kappa.B. An example is given of **solid-phase synthesis** of (II). In in vitro tests, I had IC50 of 1 .mu.M for I.kappa.B-kinase, while inhibiting other kinase activities (protein kinases A and C, and casein kinase) 36, 63, and 70%, resp. In the same tests, II showed IC50 of 25 .mu.M for I.kappa.B, and inhibited the other kinases 24, 7, and 17%, resp.

IT **313065-41-7P 313065-61-1P**
(prepn. and use of benzimidazole derivs. for treatment of illness)

RN 313065-41-7 HCA
CN 2-Naphthalenecarboxylic acid, 1,2,3,4-tetrahydro-2-[[[2-(4-pyridinyl)-1H-benzimidazol-4-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 313065-61-1 HCA
CN 1H-Benzimidazole-5-carboxamide, N-[2-(aminocarbonyl)-1,2,3,4-tetrahydro-2-naphthalenyl]-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)



IC ICM C07D401-04
ICS C07D401-14; C07D409-14; A61K031-415
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7, 63
IT 603-81-6P 606-18-8P 124340-93-8P 186320-01-4DP, **resin -bound** 313065-76-8P
(prepn. and use of benzimidazole derivs. for treatment of illness)
IT 313064-84-5P 313064-85-6P 313064-86-7P 313064-87-8P
313064-92-5P 313064-93-6P 313064-96-9P 313064-98-1P
313065-00-8P 313065-01-9P 313065-02-0P 313065-05-3P
313065-06-4P 313065-07-5P 313065-08-6P 313065-09-7P
313065-10-0P 313065-11-1P 313065-12-2P 313065-13-3P
313065-14-4P 313065-15-5P 313065-16-6P 313065-17-7P
313065-19-9P 313065-21-3P 313065-22-4P 313065-24-6P
313065-25-7P 313065-26-8P 313065-27-9P 313065-28-0P
313065-29-1P 313065-30-4P 313065-31-5P 313065-32-6P
313065-33-7P 313065-34-8P 313065-35-9P 313065-36-0P
313065-37-1P 313065-38-2P 313065-39-3P 313065-40-6P
313065-41-7P 313065-42-8P 313065-43-9P 313065-44-0P
313065-45-1P 313065-46-2P 313065-47-3P 313065-48-4P
313065-49-5P 313065-50-8P 313065-51-9P 313065-52-0P
313065-53-1P 313065-54-2P 313065-55-3P 313065-56-4P
313065-57-5P 313065-58-6P 313065-59-7P 313065-60-0P
313065-61-1P 313065-62-2P 313065-63-3P 313065-64-4P
313065-65-5P 313065-66-6P 313065-67-7P 313065-68-8P
313065-69-9P 313065-71-3P 313065-72-4P 313065-73-5P
313065-74-6P 313065-81-5P 313065-84-8P 313065-88-2P
313065-90-6P 313065-92-8P 313065-93-9P 313065-94-0P
313065-95-1P 313065-96-2P 313065-98-4P 313065-99-5P
313066-00-1P 313066-01-2P 313066-02-3P 313066-03-4P
313066-05-6P 313066-09-0P 313066-10-3P 313066-11-4P
313066-12-5P
(prepn. and use of benzimidazole derivs. for treatment of illness)

L44 ANSWER 12 OF 36 HCA COPYRIGHT 2003 ACS
134:17694 Synthesis and conformational characterization of tethered, self-complexing 1,5-dialkoxynaphthalene/1,4,5,8-naphthalenetetracarboxylic diimide systems. Zych, Andrew J.; Iverson, Brent L. (Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, 78712, USA). Journal of

the American Chemical Society, 122(37), 8898-8909 (English) 2000. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 134:17694. Publisher: American Chemical Society.

AB Chemists are beginning to explore the abiotic folding of synthetic chains, and the term "foldamers" has been used to characterize oligomers with a strong inclination to adopt specific, compact conformations. The characterization of folded structure in soln. is one of the difficult challenges facing the foldamer field. Aedamers were the first foldamers to make use of arom.-arom. interactions in water to direct folding and were designed to have several spectroscopic handles with which to probe folding conformations in soln. Herein is reported the synthesis and spectroscopic characterization of eleven aedamer dimers, with linkers chosen to provide a spectrum of lengths and flexibilities. The dimers, composed of one electron rich (1,5-dialkoxynaphthalene) and one electron deficient (1,4,5,8-naphthalenetetracarboxylic diimide) arom. group tethered by a linker, are the smallest aedamer folding unit. The powerful spectroscopic handles assocd. with the stacked aedamer groups were exploited in a comprehensive spectroscopic anal. of conformation that included UV-vis absorption spectroscopy, fluorescence measurements (including time-resolved studies), as well as detailed NMR studies. The spectra were interpreted in the context of mol. modeling/spectral prediction and structural models were developed for the different dimers in aq. soln. In most instances, the obsd. data was best described by an ensemble of predicted structures as opposed to one or few conformers. Thus, in the case of these aedamer dimers, "folding" does not appear to imply a two-state model with a rigid, unique conformation. Rather, the reported anal. indicates the data can best be described by a more dynamic model in which a given mol. spends its time in different folded conformations that are related by having a characteristic face-to-face stacking arrangement of the arom. units.

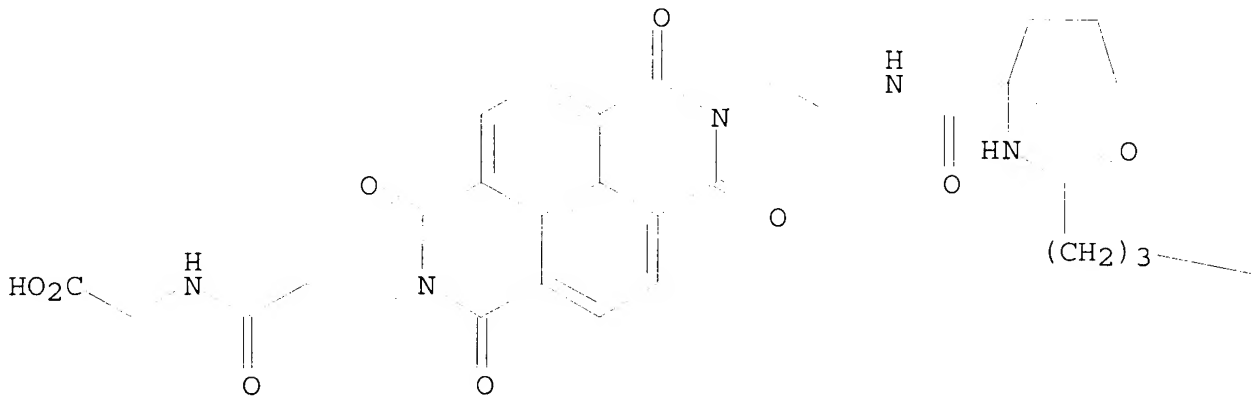
IT **309920-36-3P**
(**solid phase synthesis** and
conformation of amino acid analogs)

RN 309920-36-3 HCA

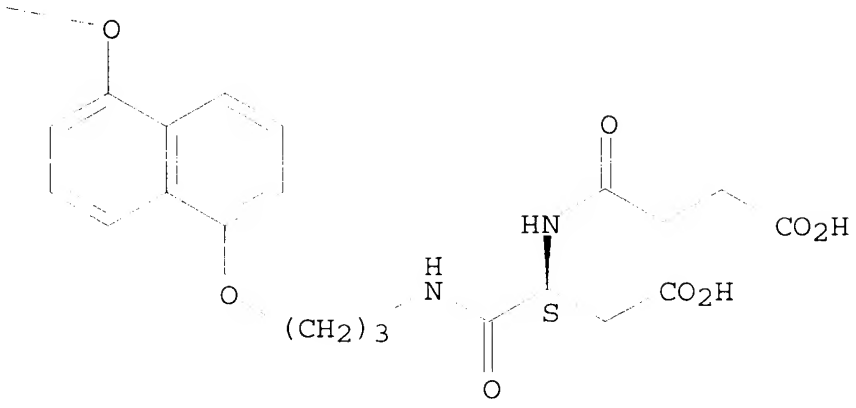
CN Glycine, N-(3-carboxy-1-oxopropyl)-L-.alpha.-aspartyl-4-[[5-(3-aminopropoxy)-1-naphthalenyl]oxy]butanoyl-1-aminocyclopentanecarbonyl-7-(2-aminoethyl)-3,6,7,8-tetrahydro-1,3,6,8-tetraoxobenzo[lmn][3,8]phenanthroline-2(1H)-propanoyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

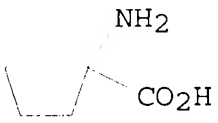
PAGE 1-A



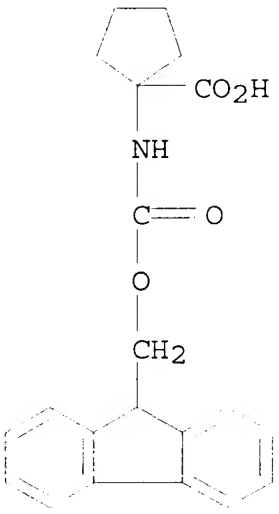
PAGE 1-B



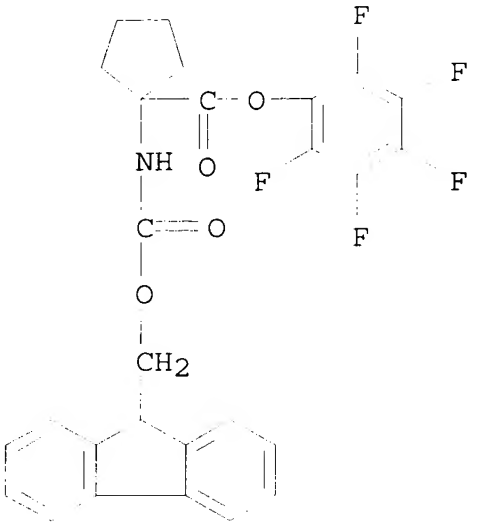
IT **52-52-8**, 1-Amino-cyclopentanecarboxylic acid
(**solid phase synthesis** and
conformation of amino acid analogs)
RN 52-52-8 HCA
CN Cyclopentanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



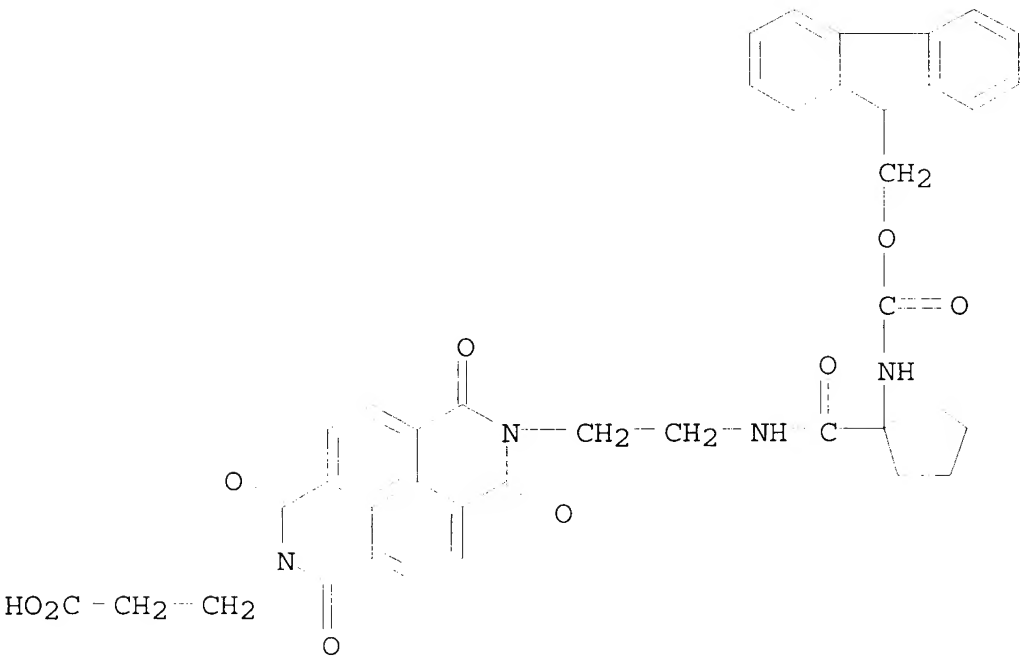
IT **117322-30-2P 309920-58-9P**
(**solid phase synthesis** and
conformation of amino acid analogs)
RN 117322-30-2 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 309920-58-9 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



IT **309920-64-7P**
(**solid phase synthesis** and
conformation of amino acid analogs)
RN 309920-64-7 HCA
CN Benzo[lmn][3,8]phenanthroline-2(1H)-propanoic acid,
7-[2-[[[1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]cyclopentyl]carbo
nyl]amino]ethyl]-3,6,7,8-tetrahydro-1,3,6,8-tetraoxo- (9CI) (CA
INDEX NAME)



CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22

ST amino acid **solid phase synthesis**
conformation folded; naphthalenetetracarboxylic diimide
dialkoxynaphthalene dimer prepn conformation mol modeling;
conformation amino acid NMR titrn NOESY UV visible fluorescence

IT Titration
(NMR; **solid phase synthesis** and
conformation of amino acid analogs)

IT UV and visible spectroscopy
(absorption; **solid phase synthesis**
and conformation of amino acid analogs)

IT Conformation
(folded; **solid phase synthesis** and
conformation of amino acid analogs)

IT Fluorescence
Molecular modeling
Overhauser spectroscopy
Solid phase synthesis
(**solid phase synthesis** and
conformation of amino acid analogs)

IT Amino acids, **preparation**
(**solid phase synthesis** and
conformation of amino acid analogs)

IT 194991-94-1
(**solid phase synthesis** and
conformation of amino acid analogs)

IT 164932-90-5P 309920-32-9P 309920-33-0P 309920-34-1P
309920-35-2P **309920-36-3P** 309920-37-4P 309920-38-5P
309920-39-6P 309920-40-9P 309920-41-0P 309920-42-1P
309920-44-3P 309920-47-6P
(**solid phase synthesis** and
conformation of amino acid analogs)

IT **52-52-8**, 1-Amino-cyclopentanecarboxylic acid 81-30-1
83-56-7, 1,5-Dihydroxynaphthalene 498-94-2, Piperidine-4-
carboxylic acid 771-61-9, Pentafluorophenol 1791-13-5
2615-15-8 5292-43-3, tert-Butyl bromoacetate 18370-81-5,
3-Bromo-propylamine 24424-99-5, Di-tert-butyl dicarbonate
35737-10-1 61895-53-2 86060-90-4 86061-01-0 88744-04-1
110661-91-1
(**solid phase synthesis** and
conformation of amino acid analogs)

IT 39160-70-8P 42749-28-0P 83948-53-2P 86770-69-6P
117322-30-2P 199126-05-1P 199126-09-5P 309920-52-3P
309920-58-9P 309920-60-3P 309920-70-5P 309920-72-7P
309920-74-9P 309920-76-1P 309920-78-3P 309920-79-4P
(**solid phase synthesis** and
conformation of amino acid analogs)

IT 194991-96-3P 199126-14-2P 309920-55-6P **309920-64-7P**
309920-66-9P 309920-68-1P
(**solid phase synthesis** and
conformation of amino acid analogs)

L44 ANSWER 13 OF 36 HCA COPYRIGHT 2003 ACS
133:282040 N-Fmoc-dehydroalanine: a versatile molecular scaffold for the rapid **solid-phase synthesis** of cycloaliphatic amino acids. Burkett, B. A.; Chai, C. L. L. (Research School of Chemistry, Australian National University, Canberra, 0200, Australia). Tetrahedron Letters, 41(34), 6661-6664 (English) 2000. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

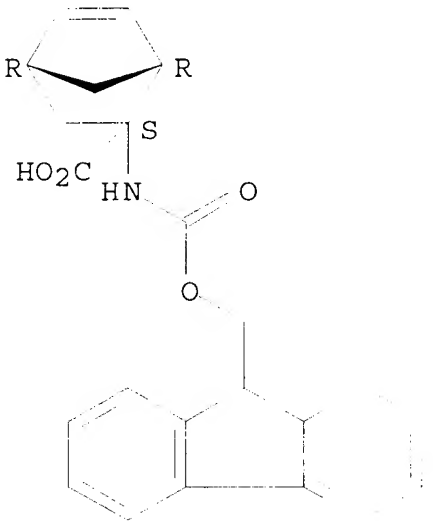
AB The synthesis of polymer-supported N-Fmoc-dehydroalanine starting from S-protected cysteine via an oxidn./elimination strategy is described. Cycloaddn. with a range of dienes afforded a range of conformationally constrained amino acids in moderate yields. The potential applications of this methodol. to combinatorial libraries is discussed.

IT **299966-33-9D, resin-bound**
(N-Fmoc-dehydroalanine as versatile mol. scaffold for rapid **solid-phase synthesis** of cycloaliph. amino acids)

RN 299966-33-9 HCA

CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

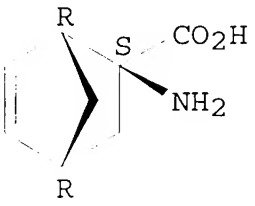


IT **76637-59-7DP, resin-bound**
(N-Fmoc-dehydroalanine as versatile mol. scaffold for rapid **solid-phase synthesis** of cycloaliph. amino acids)

RN 76637-59-7 HCA

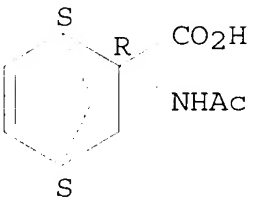
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-amino-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



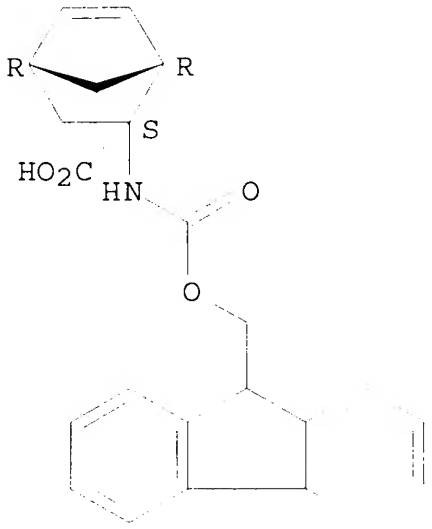
IT **133007-78-0P 299966-33-9DP, resin-bound 299966-34-0P 299966-35-1P 299966-36-2P 299966-37-3P**
(N-Fmoc-dehydroalanine as versatile mol. scaffold for rapid **solid-phase synthesis** of cycloaliph. amino acids)
RN 133007-78-0 HCA
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-(acetylamino)-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

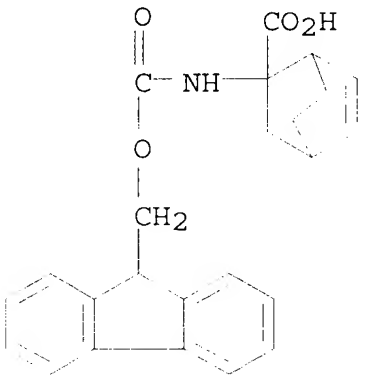


RN 299966-33-9 HCA
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

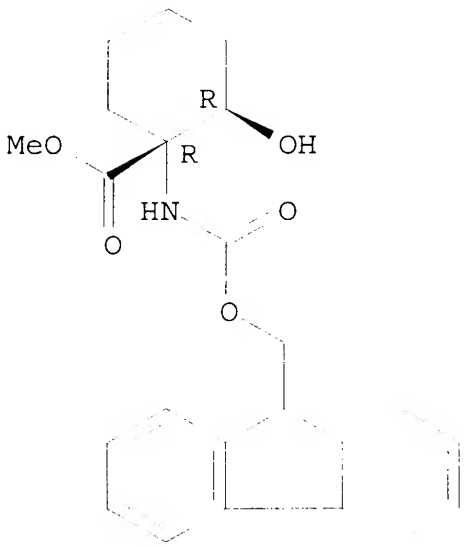


RN 299966-34-0 HCA
CN Bicyclo[2.2.2]oct-5-ene-2-carboxylic acid, 2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



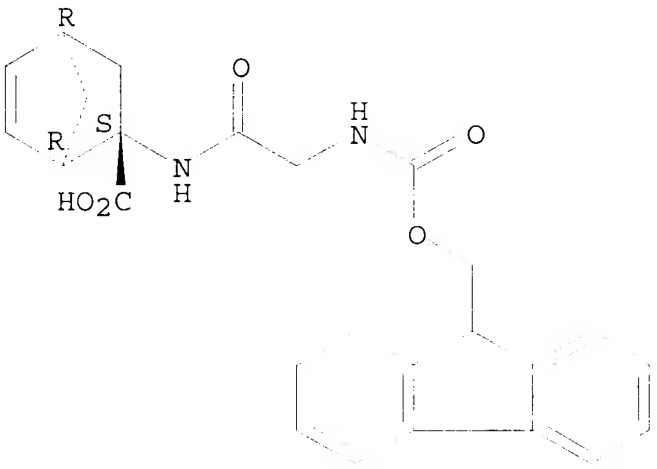
RN 299966-35-1 HCA
CN 3-Cyclohexene-1-carboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-6-hydroxy-, methyl ester, (1R,6R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



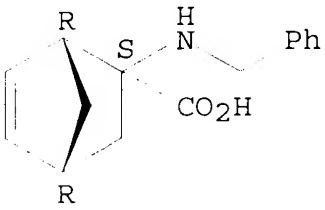
RN 299966-36-2 HCA
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-[[[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]acetyl]amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 299966-37-3 HCA
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-[(phenylmethyl)amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 34-2 (Amino Acids, Peptides, and Proteins)
ST dehydroalanine **prepn** synthon **solid phase synthesis** cycloaliph amino acid
IT **Solid phase synthesis**
Synthons
(N-Fmoc-dehydroalanine as versatile mol. scaffold for rapid **solid-phase synthesis** of cycloaliph. amino acids)
IT 100-52-7, Benzaldehyde, reactions 110-00-9, Furan 542-92-7, Cyclopentadiene, reactions 592-57-4, 1,3-Cyclohexadiene 6651-43-0 53298-33-2 **299966-33-9D, resin-bound**
(N-Fmoc-dehydroalanine as versatile mol. scaffold for rapid **solid-phase synthesis** of cycloaliph. amino acids)
IT 53298-33-2DP, **resin-bound 76637-59-7DP, resin-bound** 261522-33-2DP, **resin-bound** 299966-32-8DP, **resin-bound**
(N-Fmoc-dehydroalanine as versatile mol. scaffold for rapid **solid-phase synthesis** of cycloaliph. amino acids)
IT **133007-78-0P 299966-33-9DP, resin-bound 299966-34-0P 299966-35-1P 299966-36-2P 299966-37-3P**
(N-Fmoc-dehydroalanine as versatile mol. scaffold for rapid **solid-phase synthesis** of cycloaliph. amino acids)

L44 ANSWER 14 OF 36 HCA COPYRIGHT 2003 ACS
133:252750 Preparation of .gamma.-keto acid dipeptides as inhibitors of caspase-3. Han, Yongxin; Grimm, Erich; Aspiotis, Renee; Francoeur, Sebastien; Zamboni, Robert; Prasit, Petpiboon; Black, Cameron; Giroux, Andre; Bayly, Christopher; McKay, Daniel (Merck Frosst Canada & Co., Can.). PCT Int. Appl. WO 2000055127 A1 20000921, 146 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2.

APPLICATION: WO 2000-CA272 20000313. PRIORITY: US 1999-PV124622 19990316.

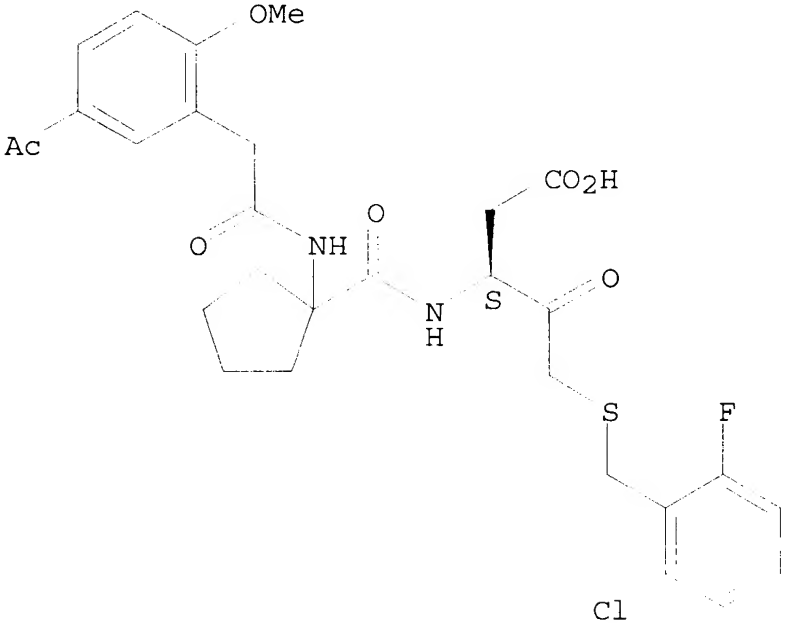
AB .gamma.-Keto acid dipeptides R(CR32)mCONHCR1R2CONHCH(CH2CO2H)COCH2S(O)n(CH2)aZ [a = 0 or 1; m, n = 0-2; Z = (un)substituted alkyl, cycloalkyl, Ph, naphthyl, 5- or 6-membered arom. or non-arom. ring or benzo-fused analogs contg. 1-3 heteroatoms selected from O, S and N; R = (un)substituted phenyl; R1 = H, aryl, alkyl, hydroxy-, alkoxy- or benzyloxyalkyl, cycloalkyl or oxa-, thia- or azacycloalkyl; R2 = H or R1R2N is a 4-7 membered ring contg. O, S or N; R3 = H, alkyl, oxo- or dioxoalkyl, alkoxy, or halo] were prepd. as inhibitors of caspase-3. Thus, (3S)-5-(benzylthio)-3-[[(2S)-2-[[2-(2,5-dimethoxyphenyl)acetyl]amino]-3-methylbutanoyl]amino]-4-oxopentanoic acid was **prepd.** by the **solid phase** method by loading (S)-FmocNHCH(CH2CO2Bu-t)COCH2Br (Fmoc = fluorenylmethoxycarbonyl) (**prepn.** described) onto a **solid support** using the technol. described by Webb et al. (1992).

IT **294859-09-9P**
(prepn. of .gamma.-keto acid dipeptides as inhibitors of caspase-3)

RN 294859-09-9 HCA

CN Pentanoic acid, 3-[[[1-[[(5-acetyl-2-methoxyphenyl)acetyl]amino]cyclopentyl]carbonyl]amino]-5-[[(2-chloro-6-fluorophenyl)methyl]thio]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07C323-59
ICS C07D239-34; C07D271-06; A61K031-198; A61P025-00

CC 34-3 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1, 7

ST peptide di keto acid prepn inhibitor caspase 3; keto acid dipeptide **solid phase synthesis** inhibitor caspase 3

IT 294860-44-9P 294860-46-1DP, **resin-bound** 294860-47-2DP, **resin-bound** 294860-48-3DP, **resin-bound** 294860-49-4P 294860-50-7P 294860-51-8P 294860-52-9P 294860-53-0DP, **resin-bound** 294860-55-2DP, **resin-bound** 294860-56-3DP, **resin-bound** 294860-57-4P 294860-59-6P 294860-60-9DP, **resin-bound** 294860-62-1P 294860-63-2P 294860-64-3P 294860-65-4P 294860-66-5P 294860-67-6P 294860-68-7P 294860-70-1P 294860-72-3P 294860-74-5P 294860-76-7P 294860-78-9P 294860-80-3P 294860-82-5P 294860-84-7P 294860-86-9P 294860-88-1P 294860-90-5P 294860-92-7P 294860-95-0P 294860-96-1P 294860-98-3P 294861-00-0P
(prepn. of .gamma.-keto acid dipeptides as inhibitors of caspase-3)

IT 294858-38-1P 294858-40-5P 294858-42-7P 294858-44-9P 294858-46-1P 294858-49-4P 294858-53-0P 294858-57-4P 294858-61-0P 294858-63-2P 294858-66-5P 294858-69-8P 294858-72-3P 294858-75-6P 294858-76-7P 294858-77-8P 294858-78-9P 294858-79-0P 294858-80-3P 294858-81-4P 294858-82-5P 294858-83-6P 294858-84-7P 294858-86-9P 294858-87-0P 294858-88-1P 294858-89-2P 294858-90-5P 294858-91-6P 294858-94-9P 294858-95-0P 294858-97-2P 294858-98-3P 294858-99-4P 294859-00-0P 294859-01-1P 294859-02-2P 294859-03-3P 294859-04-4P 294859-05-5P 294859-06-6P 294859-07-7P 294859-08-8P **294859-09-9P** 294859-10-2P 294859-11-3P 294859-12-4P 294859-13-5P 294859-14-6P 294859-15-7P 294859-16-8P 294859-17-9P 294859-18-0P 294859-19-1P 294859-20-4P 294859-21-5P 294859-22-6P 294859-23-7P 294859-24-8P 294859-25-9P 294859-26-0P 294859-27-1P 294859-28-2P 294859-29-3P 294859-30-6P 294859-31-7P 294859-32-8P 294859-33-9P 294859-34-0P 294859-35-1P 294859-36-2P 294859-37-3P 294859-38-4P 294859-39-5P 294859-40-8P 294859-41-9P 294859-43-1P 294859-45-3P 294859-47-5P 294859-49-7P 294859-51-1P 294859-53-3P 294859-54-4P 294859-56-6P 294859-58-8P 294859-60-2P 294859-62-4P 294859-64-6P 294859-66-8P 294859-68-0P 294859-70-4P 294859-72-6P 294859-74-8P 294859-76-0P 294859-79-3P 294859-82-8P 294859-85-1P 294859-88-4P 294859-89-5P 294859-91-9P 294859-93-1P 294859-95-3P 294859-97-5P 294859-98-6P 294859-99-7P 294860-00-7P 294860-01-8P 294860-02-9P 294860-03-0P 294860-04-1P 294860-05-2P 294860-06-3P 294860-07-4P 294860-08-5P 294860-09-6P 294860-10-9P 294860-12-1P 294860-13-2P 294860-14-3P 294860-15-4P 294860-16-5P 294860-17-6P 294860-18-7P 294860-19-8P 294860-20-1P 294860-21-2P 294860-22-3P 294860-23-4P 294860-24-5P 294860-25-6P 294860-26-7P 294860-27-8P

294860-28-9P 294860-29-0P 294860-30-3P 294860-31-4P
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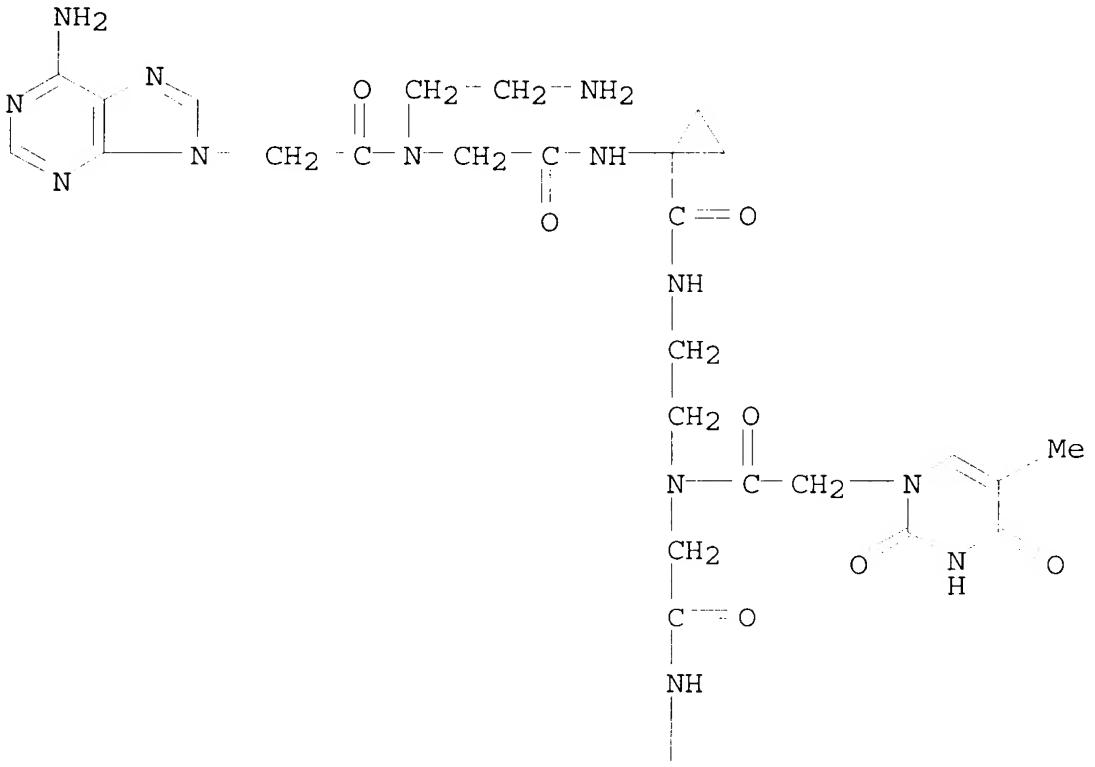
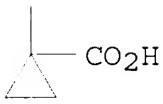
294860-36-9P 294860-37-0P 294860-38-1P 294860-39-2P
294860-40-5P 294860-41-6P 294860-42-7P 294860-43-8P
294861-08-8P 294861-11-3P 294861-13-5P
(prepn. of .gamma.-keto acid dipeptides as inhibitors of caspase-3)

L44 ANSWER 15 OF 36 HCA COPYRIGHT 2003 ACS
133:208182 Synthesis of cyclic peptide hybrids with amino acid and nucleobase side-chains. Planas, Marta; Bardaji, Eduard; Barany, George (Department of Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA). Tetrahedron Letters, 41(21), 4097-4100 (English) 2000. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 133:208182. Publisher: Elsevier Science Ltd..
AB Head-to-tail cyclic peptides with hybrid side-chains were **synthesized** by **solid-phase** assembly of the linear sequences, followed by 7-azabenzotriazol-1-yl-N-oxytrispyrrolidninophosphonium hexafluorophosphate/7-aza-1-hydroxybenzotriazole/EtN(CHMe2)2-mediated cyclization either while **resin-bound** or, after cleavage, in soln.
IT **289722-36-7P**
(synthesis of cyclic peptide hybrids with amino acid and nucleobase side-chains)
RN 289722-36-7 HCA
CN Cyclopropanecarboxylic acid, 1-[[[[2-[[[1-[[[(2-aminoethyl)[(6-amino-9H-purin-9-yl)acetyl]amino]acetyl]amino]cyclopropyl]carbonyl]amino]ethyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



CC 34-3 (Amino Acids, Peptides, and Proteins)
IT 289722-28-7P 289722-29-8P 289722-31-2P 289722-32-3P
289722-33-4P 289722-34-5P 289722-35-6P **289722-36-7P**
(synthesis of cyclic peptide hybrids with amino acid and nucleobase side-chains)

L44 ANSWER 16 OF 36 HCA COPYRIGHT 2003 ACS
133:43814 Preparation of peptides as procollagen C-proteinase inhibitors. Dankwardt, Sharon Marie; Van Wart, Harold Edgar; Walker, Keith Adrian Murray (F. Hoffmann-La Roche A.-G., Switz.). PCT Int. Appl. WO 2000034313 A1 20000615, 78 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN,

MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-EP9519 19991206. PRIORITY: US 1998-PV111661 19981210.

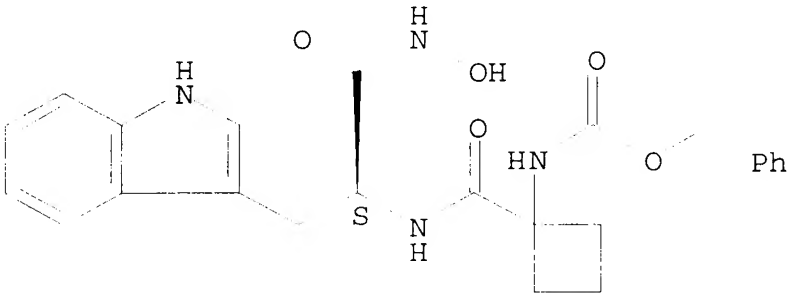
AB Peptides R7-Z-An-NR6CR4R5CONR3CR1R2CONHOH [R1, R3, R4 = H, alkyl; R2 = cycloalkyl, cycloalkylalkyl, aryl, aralkyl, aralkenyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heterocyclyl, heterocycloalkyl, or -(alkylene)-B-X, where B = O, NR8 (R8 = H, alkyl), S, SO, SO2, CO, CONR8, NR8CO2, NR8SO2, C(:NR8)NR8SO2, NR8CO and X = cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl or R2 and R3 form an alkylene or heteroalkylene chain; R6 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl; R5 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, aralkenyl, heteroaryl, heteroaralkyl, heteroaralkenyl, heterocycloalkyl, heteroalkyl, or -(alkylene)-CO-X1, where X1 = alkyl, OH, alkoxy, aryl, aralkyl, aryloxy, aralkyloxy, heteroaryl, heteroaryloxy, heteroaralkyloxy, or amino group or R5 and R4 or R5 and R6 form an alkylene group; n = 0 or 1; A = COCHR9(CH2)mNR10, where m = 0-5, R9 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocycloalkyl, or -(alkylene)-CO-X1 and R10 = H, alkyl, aralkyl, or heteroaralkyl; Z = Y-B, where Y = alkylene or a bond and B = CO, CO2, CONR8, SO2, SO2NR8, (un)substituted alkylene, or a bond; R7 = cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, or heteroaralkyl, provided that when n = 0 and Z = SO2, R2 does not contain an imidazole group] were prepd. as procollagen C-proteinase inhibitors. General exptl. procedures are given for **solid-phase synthesis** of the claimed peptides. Compds. such as (S,S)-CbzNHCHPhCONHCH(CH2-T)CONHOH (T = 4-thiazolyl, Cbz = benzyloxycarbonyl) showed IC50 in the range 0.02 to 200 .mu.M for inhibition procollagen C-proteinase.

IT **274937-36-9P 274937-37-0P**
(prepn. of peptides as procollagen C-proteinase inhibitors)

RN 274937-36-9 HCA

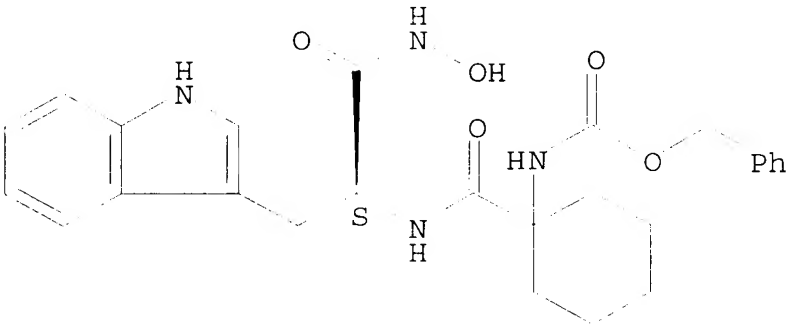
CN Carbamic acid, [1-[[[(1S)-2-(hydroxyamino)-1-(1H-indol-3-ylmethyl)-2-oxoethyl]amino]carbonyl]cyclobutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 274937-37-0 HCA
CN Carbamic acid, [1-[[[(1S)-2-(hydroxyamino)-1-(1H-indol-3-ylmethyl)-2-oxoethyl]amino]carbonyl]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07K005-06
ICS C07C259-06; C07K005-08
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1
IT **Solid phase synthesis**
(peptide; **prepn.** of peptides as procollagen C-proteinase inhibitors)

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274937-89-2P	274937-92-7P		

(prepn. of peptides as procollagen C-proteinase inhibitors)

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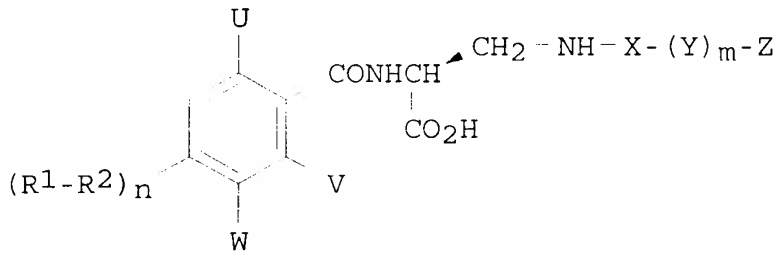
132:294010 Preparation of diaminopropionic acid derivatives as intracellular adhesion molecule-1 (ICAM-1) binding inhibitors. Fotouhi, Nader; Gillespie, Paul; Guthrie, Robert William; Pietranico-Cole, Sherrie Lynn; Yun, Weiya (F. Hoffmann-La Roche A.-G., Switz.). PCT Int. Appl. WO 2000021920 A1 20000420, 259 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,

ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-EP7620 19991012. PRIORITY: US 1998-PV104120 19981013.

GI



I

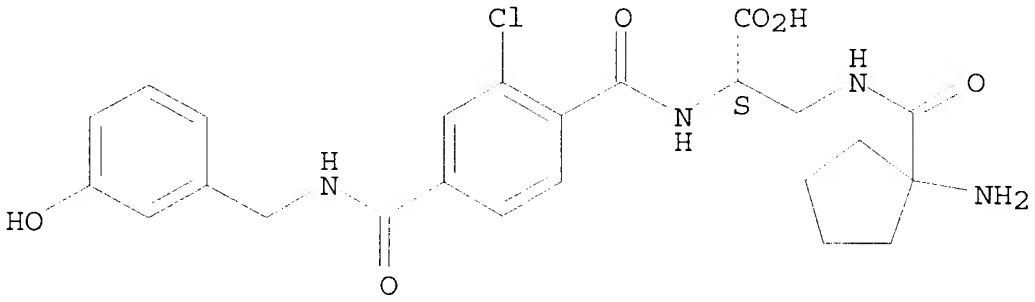
AB Diaminopropionic acid derivs. I [R1 = substituted 1-naphthyl, 4-indolyl, 4-benzimidazolyl, 4-benzodiazolyl, 4-benzotriazolyl, or phenyl; R2 = CHR3NHCO (R3 = H, carboxy, alkyl), CH2CH2CO, 1,2-cyclopropanediylcarbonyl, OCH2CO, CH:CHCHR3, CH2CH2CH(OH), CONHCHR3, or CH2NH-5,1-tetrazolediyl; U, V, W = H, halo, alkyl provided that U and V are not both hydrogen; X = CO, phenylalkylene, sulfonyl; Y = alkylene which may be substituted by amino or cycloalkyl, alkenylene, alkylenethio; Z = H, alkylthio, CO2H, CONH2, 1-adamantyl, diphenylmethyl, 3-[[(5-chloro-2-pyridinyl)amino]carbonyl]-2-pyrazinyl, hydroxy, phenylmethoxy, 2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]phenyl, [(2,6-dichlorophenyl)methoxy], Ph, (un)substituted cycloalkyl or aryl or fused ring system which may contain 0-3 heteroatoms; m, n = 0, 1] or their pharmaceutically acceptable salts or esters were prepd. and are useful for treating rheumatoid arthritis, psoriasis, multiple sclerosis, Crohn's disease, ulcerative colitis, atherosclerosis, restenosis, pancreatitis, transplant rejection, delayed graft function and diseases of ischemia reperfusion injury, including acute myocardial infarction and stroke. Thus, N-[2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]benzoyl]-3-(3-methoxybenzoylamino)-L-alanine was **prepd**. by the **solid-phase** method and showed IC50 = 1.2 nM in the LFA-1 (lymphocyte function-assocd. antigen-1)/ICAM-1 protein-protein assay.

IT **264274-97-7P 264275-18-5P**
(prepn. of diaminopropionic acid derivs. as intracellular adhesion mol.-1 (ICAM-1) binding inhibitors)

RN 264274-97-7 HCA

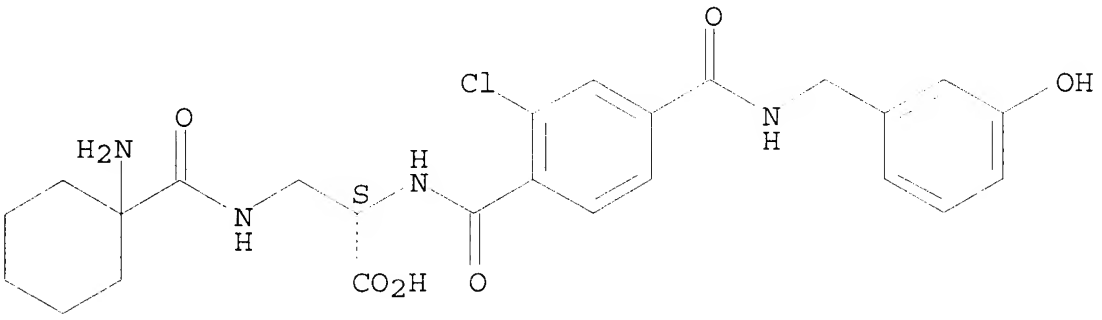
CN L-Alanine, 3-[[(1-aminocyclopentyl)carbonyl]amino]-N-[2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

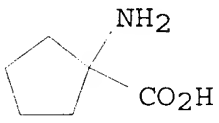


RN 264275-18-5 HCA
CN L-Alanine, 3-[[(1-aminocyclohexyl)carbonyl]amino]-N-[2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]benzoyl]- (9CI) (CA INDEX NAME)

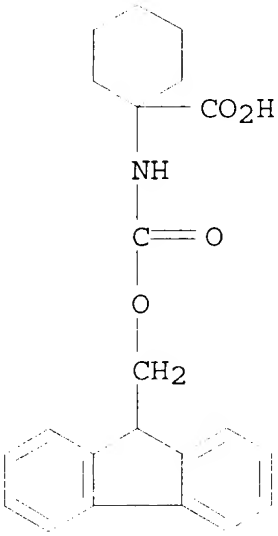
Absolute stereochemistry.



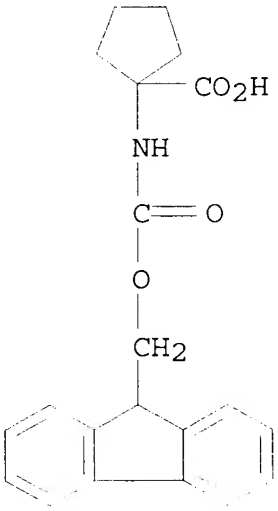
IT **52-52-8**, 1-Amino-1-cyclopentanecarboxylic acid
162648-54-6
(prepn. of diaminopropionic acid derivs. as intracellular adhesion mol.-1 (ICAM-1) binding inhibitors)
RN 52-52-8 HCA
CN Cyclopentanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 162648-54-6 HCA
CN Cyclohexanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



IT **117322-30-2P**
(prepn. of diaminopropionic acid derivs. as intracellular adhesion mol.-1 (ICAM-1) binding inhibitors)
RN 117322-30-2 HCA
CN Cyclopentanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



IC ICM C07C235-52
ICS C07C233-83; C07D333-40; C07D333-38; C07D249-18; C07D209-08; A61K031-166; A61K031-33; A61P007-00; C07C233-63; C07D213-56; C07C233-78
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264275-61-8P
(prepn. of diaminopropionic acid derivs. as intracellular adhesion mol.-1 (ICAM-1) binding inhibitors)

IT 50-30-6, 2,6-Dichlorobenzoic acid 50-78-2, Acetylsalicylic acid 50-85-1 51-36-5, 3,5-Dichlorobenzoic acid **52-52-8**, 1-Amino-1-cyclopentanecarboxylic acid 59-67-6, Nicotinic acid, reactions 62-23-7, 4-Nitrobenzoic acid 65-86-1, Orotic acid 69-72-7, Salicylic acid, reactions 74-11-3, 4-Chlorobenzoic acid 75-98-9 77-55-4, 1-Phenyl-1-Cyclopentanecarboxylic acid 79-31-2, Isobutyric acid 86-55-5, 1-Naphthoic acid 87-64-9, 2-Chloro-6-methylphenol 88-13-1, 3-Thiophenecarboxylic acid 88-14-2, 2-Furoic acid 88-65-3, 2-Bromobenzoic acid 89-77-0, 2-Amino-4-chlorobenzoic acid 93-07-2, 3,4-Dimethoxybenzoic acid 93-09-4, 2-Naphthoic acid 93-10-7, 2-Quinolinecarboxylic acid 96-98-0, 4-Methyl-3-nitrobenzoic acid 98-89-5, Cyclohexanecarboxylic acid 98-97-5, 2-Pyrazinecarboxylic acid 98-98-6, Picolinic acid 99-04-7, m-Toluic acid 99-05-8, 3-Aminobenzoic acid 99-06-9, 3-Hydroxybenzoic acid, reactions 99-10-5, 3,5-Dihydroxybenzoic acid 99-34-3 99-64-9, 3-Dimethylaminobenzoic acid 100-09-4, 4-Methoxybenzoic acid 100-52-7, Benzaldehyde, reactions 100-97-0, reactions 103-82-2, Phenylacetic acid, reactions 104-01-8, 4-Methoxyphenylacetic acid 104-03-0, 4-Nitrophenylacetic acid 117-34-0, Diphenylacetic acid 118-41-2, 3,4,5-Trimethoxybenzoic acid, reactions 118-91-2, 2-Chlorobenzoic acid 121-92-6, 3-Nitrobenzoic acid 138-41-0, 4-Carboxybenzenesulfonamide 144-90-1, 3-Aminoisobutyric acid 300-57-2, Allylbenzene 328-80-3 351-35-9, 3-Trifluoromethylphenylacetic acid 434-75-3, 2-Chloro-6-fluorobenzoic acid 446-17-3, 2,4,5-Trifluorobenzoic acid 454-92-2, 3-(Trifluoromethyl)benzoic acid 455-38-9, 3-Fluorobenzoic acid 455-40-3, 3,5-Difluorobenzoic acid 486-73-7, 1-Isoquinolinecarboxylic acid 486-74-8, 4-Quinolinecarboxylic acid 488-93-7, 3-Furoic acid 496-41-3, 2-Benzofurancarboxylic acid 498-94-2, 4-Piperidinecarboxylic acid 499-06-9, 3,5-Dimethylbenzoic acid 501-52-0, Hydrocinnamic acid 503-74-2, Isovaleric acid 527-72-0, 2-Thiophenecarboxylic acid 531-81-7, 3-Coumarincarboxylic acid 535-80-8, 3-Chlorobenzoic acid 541-48-0, 3-Aminobutyric acid 552-16-9, 2-Nitrobenzoic acid 579-75-9, 2-Methoxybenzoic acid 581-96-4, 2-Naphthylacetic acid 584-20-3 585-70-6, 5-Bromo-2-Furoic acid 585-76-2, 3-Bromobenzoic acid 586-30-1, 3-Hydroxy-4-methylbenzoic acid 586-38-9, 3-Methoxybenzoic acid 618-51-9, 3-Iodobenzoic acid 618-58-6, 3,5-Dibromobenzoic acid 618-84-8, 3-Amino-5-nitrobenzoic acid 619-04-5, 3,4-Dimethylbenzoic acid 619-84-1, 4-Dimethylaminobenzoic acid 619-86-3, 4-Ethoxybenzoic acid 621-37-4, 3-Hydroxyphenylacetic acid 634-97-9, 2-Pyrrolecarboxylic

acid 643-43-6, 2,4-Dinitrophenylacetic acid 645-08-9, 3-Hydroxy-4-methoxybenzoic acid 645-12-5, 5-Nitro-2-Furoic acid 645-45-4, Benzenepropanoyl chloride 696-59-3, 2,5-Dimethoxytetrahydrofuran 701-99-5 723-62-6, 9-Anthracenecarboxylic acid 828-51-3, 1-Adamantanecarboxylic acid 830-09-1, 4-Methoxycinnamic acid 873-62-1, 3-Cyanophenol 874-60-2, p-Toluoyl chloride 933-88-0, o-Toluoyl chloride 934-60-1, 6-MethylPicolinic acid 939-87-7 1123-00-8, Cyclopentaneacetic acid 1123-25-7, 1-Methyl-1-Cyclohexanecarboxylic acid 1124-65-8, 3-(2-Thienyl)acrylic acid 1132-21-4, 3,5-Dimethoxybenzoic acid 1184-90-3, Aminoiminomethanesulfonic acid 1204-75-7, 3-Hydroxy-2-quinoxalinecarboxylic acid 1447-14-9, 2,2-Dichloro-1-methylcyclopropanecarboxylic acid 1501-27-5, Monomethyl glutarate 1670-81-1, 5-Indolecarboxylic acid 1670-82-2, 6-Indolecarboxylic acid 1711-06-4, m-Toluoyl chloride 1759-53-1, Cyclopropanecarboxylic acid 1877-71-0, Monomethyl isophthalate 1877-72-1, 3-Cyanobenzoic acid 1918-77-0, 2-Thiopheneacetic acid 1918-79-2, 5-Methyl-2-thiophenecarboxylic acid 1975-50-4, 2-Methyl-3-nitrobenzoic acid 2150-44-9 2243-42-7, 2-Phenoxybenzoic acid 2386-60-9, 1-Butanesulfonyl chloride 2483-46-7 2486-70-6, 4-Amino-3-Methylbenzoic acid 2488-15-5 2510-36-3, 3,5-Dimethylisoxazole-4-carboxylic acid 2687-25-4 2942-59-8, 2-Chloronicotinic acid 3113-71-1, 3-Methyl-4-nitrobenzoic acid 3336-41-2 3400-45-1, Cyclopentanecarboxylic acid 3622-35-3, Benzothiazole-6-carboxylic acid 3685-23-2, cis-4-Amino-1-cyclohexanecarboxylic acid 3721-95-7, Cyclobutanecarboxylic acid 3724-65-0, 2-Butenoic acid 3886-70-2 4100-13-4, 1,2,3-Thiadiazole-4-carboxylic acid 4593-90-2, 3-Phenylbutyric acid 4630-80-2 4919-37-3 4940-39-0, 2-Chromonecarboxylic acid 5006-66-6, 6-Hydroxynicotinic acid 5071-96-5, 3-Methoxybenzylamine 5081-36-7, 3-Methoxy-4-nitrobenzoic acid 5292-21-7, Cyclohexaneacetic acid 5326-23-8, 6-Chloronicotinic acid 5329-14-6, Sulfamic acid 5372-81-6 6120-95-2, 1-Phenyl-1-cyclopropanecarboxylic acid 6284-80-6, 9-Fluoreneacetic acid 6307-83-1, 3-Bromo-5-nitrobenzoic acid 6314-28-9, Benzo[b]thiophene-2-carboxylic acid 6324-10-3, 4,5-Dibromo-2-thiophenecarboxylic acid 6480-68-8, 3-Quinolinecarboxylic acid 6482-24-2, 2-Bromoethyl methyl ether 7311-63-9, 5-Bromo-2-thiophenecarboxylic acid 7311-64-0, 3-Bromo-2-thiophenecarboxylic acid 7409-18-9, 3-Nitrobenzylamine 7536-55-2 7697-28-1, 4-Bromo-3-Methylbenzoic acid 10351-19-6, 4-Pyridylthioacetic acid 13139-14-5 13726-67-5 13734-34-4 15733-83-2, 4-Methoxy-2-Quinolinecarboxylic acid 15761-39-4 15788-16-6, Benzimidazole-5-carboxylic acid 15872-41-0, 4-Pentyloxybenzoic acid 16136-52-0, 1h-Indole-4-carbonitrile 16179-97-8, 2-Pyridineacetic acid hydrochloride 16727-43-8, 2,6-Dimethoxynicotinic acid 18212-21-0, 4-Methyl-1,2,3-Thiadiazole-5-carboxylic acid 18643-84-0 18643-86-2 19337-97-4, trans-3-(3-Pyridyl)acrylic acid 21169-71-1, 5-Isoxazolecarboxylic acid 21461-84-7 21905-86-2, 4-Cinnolinecarboxylic acid 23806-24-8, 3-Methyl-2-thiophenecarboxylic acid 23814-12-2,

5-Benzotriazolecarboxylic acid 23945-44-0, 2,4-Dihydroxy-5-pyrimidinecarboxylic acid 24065-33-6, 5-Chloro-2-thiophenecarboxylic acid 24277-39-2 25026-64-6 26371-07-3, 1-Piperidinepropanoic acid 27527-05-5 34967-24-3, 3,5-Dimethoxybenzylamine 35661-39-3 35661-60-0 37642-33-4 38186-54-8, 1,2,3,4-Tetrahydro-9-acridinecarboxylic acid 43200-83-5 51762-52-8 53137-27-2, 2,4-Dimethyl-5-thiazolecarboxylic acid 53440-12-3, 1,2,3,4-Tetrahydro-2-naphthalenecarboxylic acid 59337-89-2, 3-Chloro-2-thiophenecarboxylic acid 59748-90-2, 4-Bromo-2-chlorobenzoic acid 63094-36-0 71050-40-3, 4-Methoxy-3-thiophenecarboxylic acid 71989-33-8 73604-31-6, 3-Hydroxybenzylamine 74385-09-4 77128-70-2 77284-32-3 78348-24-0, 2-Indolinecarboxylic acid 79990-15-1 83647-42-1, 3-Amino-2-methylbenzyl alcohol 83792-48-7 84000-07-7 88050-17-3 88574-07-6 88768-45-0, 2-(Pyrimidylthio)acetic acid 94744-50-0 95753-55-2 97945-19-2 99780-96-8 102410-65-1 112402-12-7 112883-29-1 114559-25-0 116423-07-5 116821-47-7 121023-47-0 133054-21-4 133659-14-0 134098-70-7 145623-04-7 161622-05-5, 3-Fluoro-5-(trifluoromethyl)benzoic acid **162648-54-6** 167690-53-1 185116-42-1 198348-89-9 204322-11-2 204322-23-6 264276-40-6 264276-41-7 264276-42-8

(prepn. of diaminopropionic acid derivs. as intracellular adhesion mol.-1 (ICAM-1) binding inhibitors)

IT 1074-85-7P, 1H-Indole-4-methanol 3468-18-6P, 1H-Indole-4-methanamine 4481-28-1P 4887-83-6P, 4-Methylbenzimidazole 10388-19-9P, 3-Iodobenzamide 13269-15-3P 25912-50-9P 28875-17-4P, Boc ala ome 33617-41-3P 35458-34-5P 39830-66-5P 88443-77-0P, 3-Acetoxyphenylacetic acid 99548-55-7P 107356-10-5P 116934-87-3P **117322-30-2P** 122235-70-5P 132873-77-9P 139525-24-9P 143468-76-2P 147900-45-6P 148842-87-9P 148928-15-8P 160833-27-2P 186320-18-3P 186320-19-4P 188970-92-5DP, **resin-bound** 194471-84-6P 194471-86-8P 214759-51-0P 214759-52-1P 220848-41-9P 220848-42-0P 220848-45-3P 220848-47-5P 220876-15-3P 245466-16-4DP, **resin-bound** 264272-63-1P 264272-64-2P 264272-65-3P 264272-66-4P 264272-67-5P 264272-68-6P 264272-69-7P 264272-70-0P 264272-71-1P 264272-72-2P 264272-73-3P 264272-74-4P 264272-75-5P 264272-76-6P 264272-77-7P 264272-78-8P 264272-79-9P 264272-80-2P 264272-81-3P 264272-82-4P 264272-83-5P 264272-84-6P 264272-85-7P 264272-86-8P 264272-87-9P 264272-88-0P 264272-89-1P 264272-90-4P 264272-91-5P 264272-92-6P 264272-93-7P 264272-94-8P 264272-95-9P 264272-96-0P 264272-97-1P 264272-98-2P 264272-99-3P 264273-00-9P 264273-01-0P 264273-02-1P 264273-03-2P 264273-04-3P 264273-05-4P 264273-06-5P 264273-07-6P 264273-08-7P 264273-09-8P 264273-10-1P 264273-11-2DP, **resin-bound** 264273-12-3DP, **resin-bound** 264273-13-4DP, **resin-bound** 264273-14-5DP, **resin-bound** 264273-15-6DP, **resin-bound** 264273-16-7DP, **resin-**

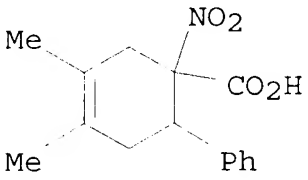
bound 264273-17-8P 264273-18-9P 264273-19-0P
264273-20-3P 264276-06-4DP, **resin-bound**
264276-09-7DP, **resin-bound** 264276-09-7P
264276-13-3P 264276-14-4P 264276-15-5P 264276-16-6P
264276-17-7P 264276-18-8P 264276-19-9P 264276-20-2P
264276-21-3P 264276-22-4P 264276-23-5P 264276-24-6P
264276-25-7P 264276-26-8P 264276-27-9P 264276-28-0P
264276-30-4P 264276-31-5P 264276-32-6P 264276-33-7P
264276-34-8P 264276-35-9P 264276-36-0P 264276-37-1P
264276-38-2P 264276-39-3P 264276-43-9P 264276-44-0P
264276-45-1P 264276-46-2P 264276-47-3P 264276-48-4P
264276-49-5P 264276-50-8P 264276-51-9P 264276-52-0P
264276-53-1P 264276-54-2P 264276-55-3P 264276-56-4P
264276-57-5P 264276-58-6P 264276-60-0P 264276-61-1P
264276-62-2P 264276-63-3P 264276-64-4P 264276-66-6P
264276-67-7P 264276-68-8P 264276-69-9P 264276-70-2P
264276-71-3P 264276-72-4P 264276-73-5P 264276-74-6P
264276-75-7P 264276-76-8P
(prepn. of diaminopropionic acid derivs. as intracellular adhesion mol.-1 (ICAM-1) binding inhibitors)

L44 ANSWER 18 OF 36 HCA COPYRIGHT 2003 ACS
132:236583 The preparation of **resin-bound** nitro alkenes and some applications in high-pressure promoted cycloadditions. Kuster, George J.; Scheeren, Hans W. (Department of Organic Chemistry, NSR Center for Molecular Structure, Design and Synthesis, University of Nijmegen, Nijmegen, 6525 ED, Neth.). Tetrahedron Letters, 41(4), 515-519 (English) 2000. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 132:236583. Publisher: Elsevier Science Ltd..

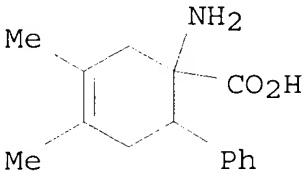
AB The prepn. of **resin-bound** nitro alkenes via a microwave-assisted Knoevenagel reaction of **resin-bound** nitro-acetic acid with aryl- and alkyl-substituted aldehydes is described. The potential of these **resin-bound** nitro alkenes for application in combinatorial chem. is demonstrated by a Diels-Alder reaction with (CH2:CMe)2 as well as 1-pot 3-component tandem [4+2]/[3+2] reactions with EtOCH:CH2 and PhCH:CH2. The cycloaddns. were promoted by high pressure.

IT **261910-77-4DP, resin-bound**
261910-79-6DP, resin-bound
(prepn. and high-pressure-promoted cycloaddn. of **resin-bound** nitro alkenes)

RN 261910-77-4 HCA
CN 3-Cyclohexene-1-carboxylic acid, 3,4-dimethyl-1-nitro-6-phenyl- (9CI) (CA INDEX NAME)



RN 261910-79-6 HCA
CN 3-Cyclohexene-1-carboxylic acid, 1-amino-3,4-dimethyl-6-phenyl- (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)
ST nitro alkene **resin bound** prepn cycloaddn; butadiene nitro alkene Diels Alder solid phase; styrene ethoxyethene nitro alkene cycloaddn solid phase
IT Alkenes, preparation
(nitro, **resin-bound**; prepn. and high-pressure-promoted cycloaddn. of **resin-bound** nitro alkenes)
IT Combinatorial chemistry
Cycloaddition reaction
Diels-Alder reaction
Solid phase synthesis
(**prepn.** and high-pressure-promoted cycloaddn. of **resin-bound** nitro alkenes)
IT 78-84-2, Isobutanal 98-01-1, 2-Furaldehyde, reactions 100-42-5, Styrene, reactions 100-52-7, Benzaldehyde, reactions 109-92-2, Ethyl vinyl ether 500-22-1, 3-Pyridinaldehyde 513-81-5, 2,3-Dimethylbutadiene 625-75-2, Nitroacetic acid 1003-29-8, 2-Pyrrolaldehyde
(prepn. and high-pressure-promoted cycloaddn. of **resin-bound** nitro alkenes)
IT 625-75-2DP, **resin-bound 261910-77-4DP**, **resin-bound 261910-79-6DP**, **resin-bound**
(prepn. and high-pressure-promoted cycloaddn. of **resin-bound** nitro alkenes)
IT 261910-78-5P 261910-80-9P 261910-81-0P 261910-82-1P 261910-83-2P 261910-84-3P 261910-85-4P
(prepn. and high-pressure-promoted cycloaddn. of **resin-bound** nitro alkenes)

L44 ANSWER 19 OF 36 HCA COPYRIGHT 2003 ACS

132:166498 Correlation between the mobility of spin-labeled peptide chains and resin solvation: an approach to optimize the synthesis of aggregating sequences. Cilli, Eduardo M.; Marchetto, Reinaldo; Schreier, Shirley; Nakaie, Clovis R. (Department of Biophysics, Universidade Federal de Sao Paulo, Sao Paulo, CEP 04044-020, Brazil). Journal of Organic Chemistry, 64(25), 9118-9123 (English) 1999. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB Resin solvation properties affect the efficiency of the coupling reactions in **solid-phase** peptide **synthesis**. Here, the authors report a novel approach to evaluate resin solvation properties, making use of spin label ESR (EPR) spectroscopy. The aggregating peptide sequences VVLGAAIV and ING were assembled in benzhydrylamine-resin with different amino group contents (up to 2.6 mmol/g) to examine the extent of chain assocn. within the beads. These model peptidyl-resins were first labeled at their N-terminus with the amino acid spin label 2,2,6,6-tetramethylpiperidine-N-oxyl-4-amino-4-carboxylic acid (Toac). Their solvation properties in different solvents were estd., either by bead swelling measurement or by assessing the dynamics of their polymeric matrixes through the anal. of Toac EPR spectra, and were correlated with the yield of the acylation reaction. In most cases the coupling rate was found to depend on bead swelling. Comparatively, the EPR approach was more effective. Line shape anal. allowed the detection of more than one peptide chain population, which influenced the reaction. The results demonstrated the unique potential of EPR spectroscopy not only for improving the yield of peptide synthesis, even in challenging conditions, but also for other relevant polymer-supported methodologies in chem. and biol.

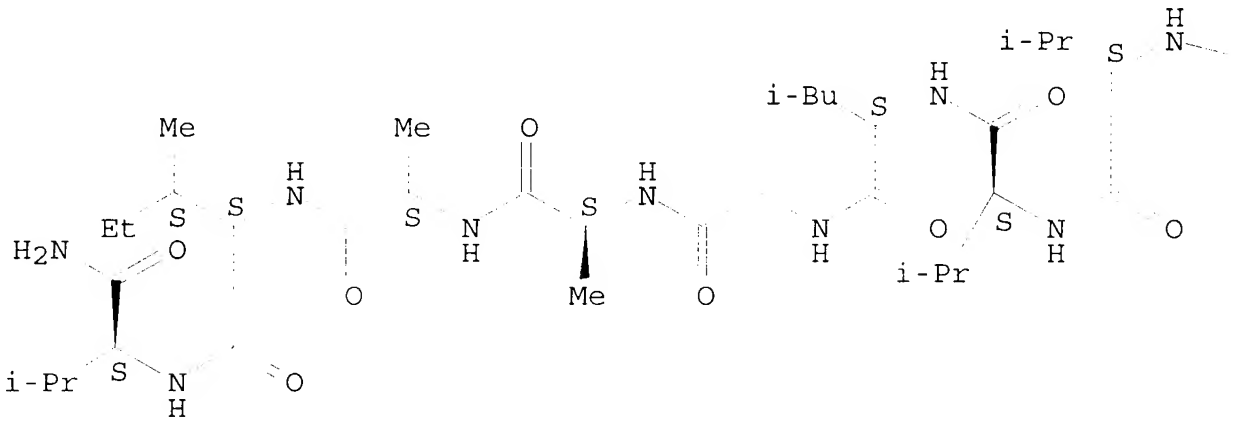
IT **258511-35-2DP**, benzhydrylamine **resin-bound**
258511-38-5DP, benzhydrylamine **resin-bound**
258511-40-9DP, benzhydrylamine **resin-bound**
(detn. of optimal **resin** solvation for solid-phase peptide coupling by studying spin-labeled, **resin-bound** peptides with EPR spectroscopy and bead swelling methods)

RN 258511-35-2 HCA

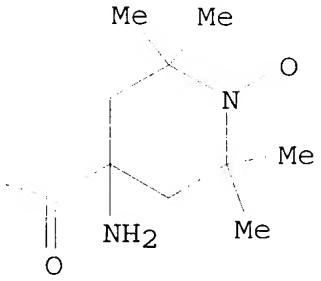
CN L-Valinamide, 4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-valyl-L-valyl-L-leucylglycyl-L-alanyl-L-alanyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

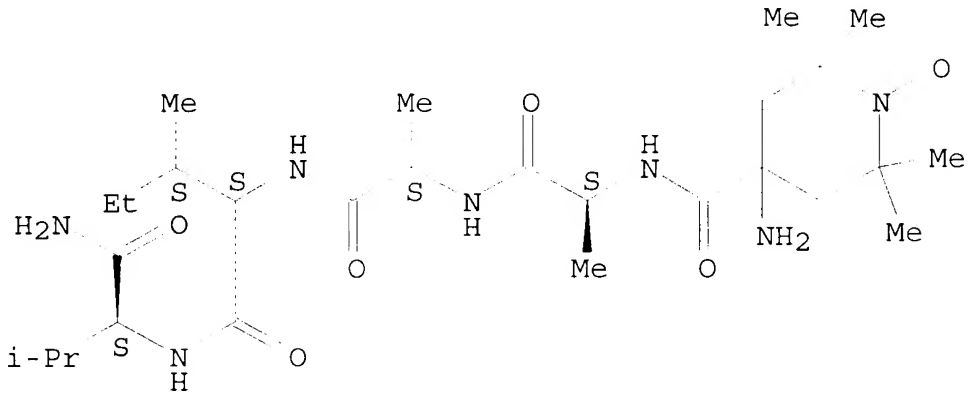


PAGE 1-B



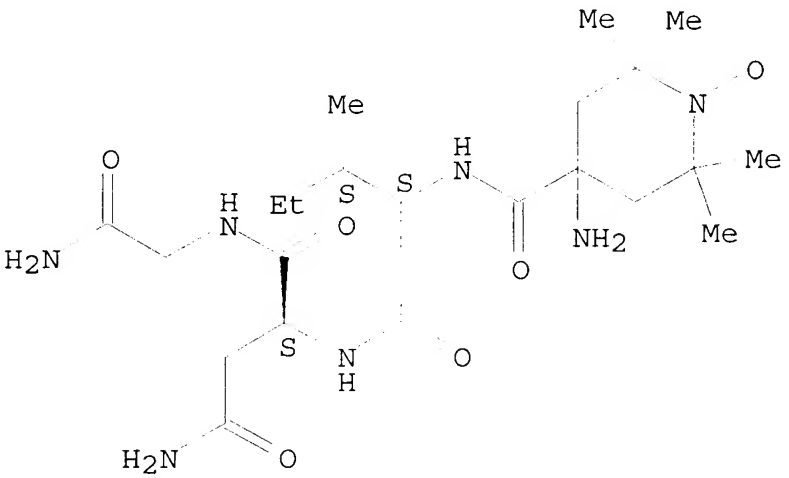
RN 258511-38-5 HCA
CN L-Valinamide, 4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-alanyl-L-alanyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 258511-40-9 HCA
CN Glycinamide, 4-amino-2,2,6,6-tetramethyl-1-oxy-4-piperidinecarbonyl-L-isoleucyl-L-asparaginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22
ST spin labeled benzhydrylamine **resin bound** peptide prepn EPR spectroscopy; peptide aggregating sequence **solid phase synthesis** optimal resin solvation
IT ESR spectroscopy
Peptide coupling
Solvation
(detn. of optimal resin solvation for solid-phase peptide coupling by studying spin-labeled, **resin-bound** peptides with EPR spectroscopy and bead swelling methods)
IT **Solid phase synthesis**
(peptide; detn. of optimal resin solvation for solid-phase

peptide coupling by studying spin-labeled, **resin-bound** peptides with EPR spectroscopy and bead swelling methods)

IT Peptides, preparation
(spin-labeled; detn. of optimal resin solvation for solid-phase peptide coupling by studying spin-labeled, **resin-bound** peptides with EPR spectroscopy and bead swelling methods)

IT 258511-37-4DP, benzhydrylamine **resin-bound**
258511-39-6DP, benzhydrylamine **resin-bound**
258511-41-0DP, benzhydrylamine **resin-bound**
(detn. of optimal **resin** solvation for solid-phase peptide coupling by studying spin-labeled, **resin-bound** peptides with EPR spectroscopy and bead swelling methods)

IT **258511-35-2DP**, benzhydrylamine **resin-bound**
258511-38-5DP, benzhydrylamine **resin-bound**
258511-40-9DP, benzhydrylamine **resin-bound**
(detn. of optimal **resin** solvation for solid-phase peptide coupling by studying spin-labeled, **resin-bound** peptides with EPR spectroscopy and bead swelling methods)

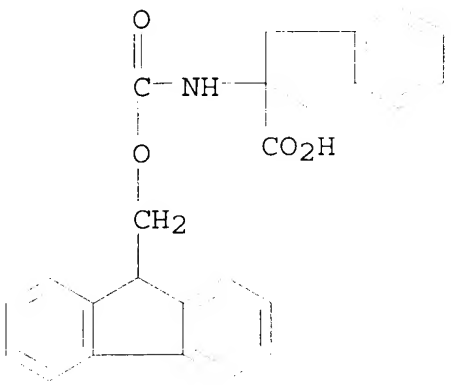
L44 ANSWER 20 OF 36 HCA COPYRIGHT 2003 ACS
132:3340 **Solid-Phase Synthesis** of 2-Aminoimidazolones. Fu, Mengmeng; Fernandez, Monica; Smith, Marie L.; Flygare, John A. (Tularik Inc., South San Francisco, CA, 94080, USA). Organic Letters, 1(9), 1351-1353 (English) 1999. CODEN: ORLEF7. ISSN: 1523-7060. OTHER SOURCES: CASREACT 132:3340. Publisher: American Chemical Society.

AB A **solid-phase** route for the **prepn.** of 2-aminoimidazolones has been developed which can incorporate diverse functionality at each position of the mol. **Resin-bound** S-Me isothioureas were converted to aminoimidazolones by using com. available Fmoc-protected amino acids. Phenylmethylene-substituted aminoimidazolones were accessed by reaction of the S-Me isothiourea with 5-substituted oxazolones.

IT **135944-07-9**
(**solid-phase synthesis** of aminoimidazolones)

RN 135944-07-9 HCA

CN 1H-Indene-2-carboxylic acid, 2-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2,3-dihydro- (9CI) (CA INDEX NAME)

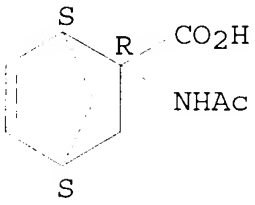


CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
ST aminoimidazolone **solid phase synthesis** ; imidazolone amino **solid phase synthesis**
IT **Solid phase synthesis**
(**solid-phase synthesis** of aminoimidazolones)
IT 842-74-0 7152-75-2 15601-44-2 29022-11-5 **135944-07-9** 186320-01-4 186320-21-8 250740-51-3 250740-52-4
(**solid-phase synthesis** of aminoimidazolones)
IT 113125-71-6P 250740-38-6P 250740-39-7P 250740-40-0P 250740-41-1P 250740-42-2P 250740-43-3P 250740-44-4P 250740-45-5P 250740-46-6P 250740-47-7P 250740-48-8P 250740-49-9P
(**solid-phase synthesis** of aminoimidazolones)

L44 ANSWER 21 OF 36 HCA COPYRIGHT 2003 ACS
131:337336 The Diels-Alder reactions of **polymer bound** dehydroalanine derivatives. Burkett, Brendan A.; Chai, Christina L. L. (Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia). Tetrahedron Letters, 40(38), 7035-7038 (English) 1999. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..
AB The synthesis and Diels-Alder cycloaddns. of a no. of **polymer bound** dehydroalanine derivs. are described. The studies compare methodologies for accessing **polymer bound** dehydroalanines and establish the versatility and efficiency of solid phase Diels-Alder reactions in the synthesis of carbocyclic amino acids. These studies nicely complement the growing repertoire of methodologies for the functionalization of amino acid derivs.
IT **133007-78-0P 249744-62-5P 249744-63-6P 249744-65-8P**
(Diels-Alder reactions of **polymer bound** dehydroalanine derivs.)

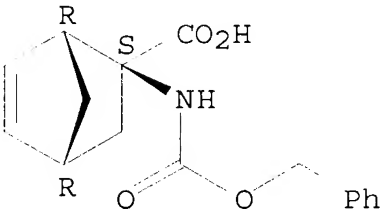
RN 133007-78-0 HCA
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-(acetylamino)-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 249744-62-5 HCA
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-[[(phenylmethoxy)carbonyl]amino]-, (1R,2S,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

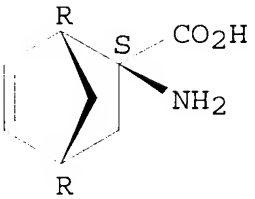


RN 249744-63-6 HCA
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-amino-, (1R,2S,4R)-rel-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

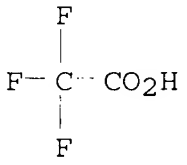
CRN 76637-59-7
CMF C8 H11 N O2

Relative stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

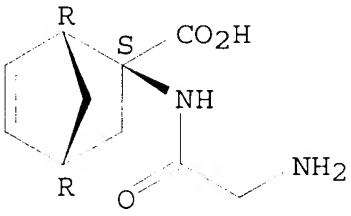


RN 249744-65-8 HCA
CN Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-[(aminoacetyl)amino]-, (1R,2S,4R)-rel-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

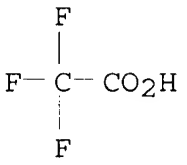
CRN 249744-64-7
CMF C10 H14 N2 O3

Relative stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



CC 34-3 (Amino Acids, Peptides, and Proteins)
ST Diels Alder **polymer bound** dehydroalanine
IT Diels-Alder reaction
Solid phase synthesis
(Diels-Alder reactions of **polymer bound** dehydroalanine derivs.)
IT 542-92-7, Cyclopentadiene, reactions

(Diels-Alder reactions of **polymer bound** dehydroalanine derivs.)

IT 5429-56-1DP, **resin-bound** 39692-63-2DP, **resin-bound** 45101-25-5DP, **resin-bound** 50333-24-9DP, **resin-bound**
(Diels-Alder reactions of **polymer bound** dehydroalanine derivs.)

IT **133007-78-0P 249744-62-5P 249744-63-6P 249744-65-8P**
(Diels-Alder reactions of **polymer bound** dehydroalanine derivs.)

L44 ANSWER 22 OF 36 HCA COPYRIGHT 2003 ACS

131:243593 Preparation of peptides as inhibitors of caspases. Wannamaker, Marion W.; Bemis, Guy W.; Charifson, Paul S.; Lauffer, David J.; Mullican, Michael D.; Murcko, Mark A.; Wilson, Keith P.; Janetka, James W.; Davies, Robert J.; Grillot, Anne-Laure; Shi, Zhan; Forster, Cornelia J. (Vertex Pharmaceuticals Incorporated, USA). PCT Int. Appl. WO 9947545 A2 19990923, 297 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US5919 19990319. PRIORITY: US 1998-PV78770 19980319.

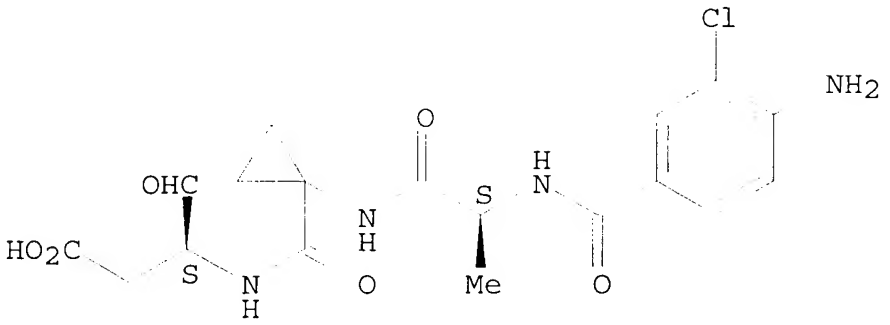
AB Peptides R1NR2XCONR4CR52CONHY [Y = CH(CHO)CH2(CH2)mCOR7, (m = 0 or 1 and R7 = OH or ester, NHOH) or cyclic lactol deriv. when R7 is OH; X = CR32 or NR3 (R3 = H, an amino acid side chain, alkyl, cycloalkyl, aryl, etc.); R1 = H, R8, COR8, COCOR8, SO2R8, SOR8, CO2R8, CONHR8, SO2NHR8, SONHR8, COCONHR8, COCH:CHR8, etc. (R8 = alkyl, cycloalkyl, aryl, etc.); R2 = H or R2 and R3 may form a ring; R4 = H and R5 = H, amino acid side chain, R8, etc. or R4 and R5 may form a ring] were prepd. as inhibitors of caspases. Thus, p-AcNHC6H4CO-L-Val-L-Pro-NHCH(CHO)CH2CO2H-(S) was **prepd**. by the **solid-phase** method and showed ki < 10 nm for inhibition of interleukin-1.beta. converting enzyme (ICE, caspase-1).

IT **244132-37-4P**
(prepn. of peptides as inhibitors of caspases)

RN 244132-37-4 HCA

CN Butanoic acid, 3-[[[1-[[(2S)-2-[(4-amino-3-chlorobenzoyl)amino]-1-oxopropyl]amino]cyclopropyl]carbonyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07K005-023
ICS A61K038-04; A61K031-47; A61K038-03; C07D401-12

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7

IT

244130-74-3P	244130-75-4P	244130-76-5P	244130-77-6P
244130-78-7P	244130-79-8P	244130-80-1P	244130-81-2P
244130-82-3P	244130-83-4P	244130-84-5P	244130-85-6P
244130-86-7P	244130-87-8P	244130-88-9P	244130-89-0P
244130-90-3P	244130-91-4P	244130-94-7P	244130-95-8P
244130-96-9P	244130-97-0P	244130-98-1P	244130-99-2P
244131-00-8P	244131-01-9P	244131-02-0P	244131-04-2P
244131-05-3P	244131-06-4P	244131-07-5P	244131-08-6P
244131-09-7P	244131-10-0P	244131-11-1P	244131-12-2P
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244134-69-8P 244134-70-1P 244134-71-2P 244134-72-3P
244134-73-4P
(prepn. of peptides as inhibitors of caspases)

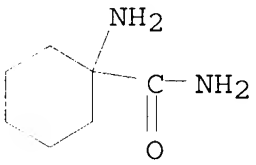
IT 56-41-7, L-Alanine, reactions 79-03-8, Propionyl chloride
96-41-3, Cyclopentanol 98-98-6, 2-Pyridinecarboxylic acid
100-07-2, p-Anisoyl chloride 100-49-2, Cyclohexylmethanol
103-80-0, Phenylacetyl chloride 108-12-3, Isovaleryl chloride
122-97-4, 3-Phenyl-1-propanol 400-76-0 486-73-7,
1-Isoquinolinecarboxylic acid 591-50-4, Iodobenzene 700-57-2,
2-Adamantanol 873-76-7, 4-Chlorobenzenemethanol 879-65-2,
2-Quinoxalinecarboxylic acid 944-43-4 2216-51-5 2486-71-7,
4-Amino-3-chlorobenzoic acid 3282-30-2, Pivaloyl chloride
3336-41-2 3637-61-4, Cyclopentylmethanol 4093-31-6 4254-29-9,
2-Indanol 4919-37-3, 3,5-Dimethyl-4-hydroxybenzoic acid
6223-83-2, 9-Oxo-4-fluorenecarboxylic acid 7206-70-4 10349-57-2,
6-Quinolinecarboxylic acid 15356-60-2 21553-46-8,
3,5-Dimethyl-4-methoxybenzoic acid 21803-75-8,
4-Amino-3-chlorobenzonitrile 26250-84-0 33300-72-0 37908-97-7,
3,5-Dichloro-4-methoxybenzoic acid 41727-45-1 56961-25-2,
3,5-Dichloro-4-aminobenzoic acid 58452-00-9, 3-Benzyloxy-4-
methoxybenzoic acid 60108-51-2 60772-67-0, 3-Isopropoxybenzoic
acid 72228-75-2 74844-91-0 103321-53-5 116939-94-7
143305-32-2 146803-45-4D, **resin-bound**
147650-70-2 192760-02-4 193945-93-6 220184-67-8 233266-69-8
244132-28-3D, **resin-bound** 244133-23-1
244133-24-2 244134-11-0 244134-14-3 244134-15-4 244134-17-6
244134-20-1 244134-21-2 244134-22-3 244134-23-4 244134-25-6
244134-26-7 244134-27-8 244134-31-4 244134-33-6 244134-36-9

244134-53-0 244134-63-2 244134-64-3
(prepn. of peptides as inhibitors of caspases)

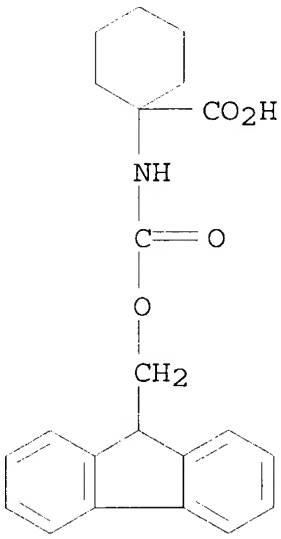
L44 ANSWER 23 OF 36 HCA COPYRIGHT 2003 ACS
131:73182 Six new photolabile linkers for **solid phase synthesis**. 2. Coupling of various building blocks and photolytic cleavage. Akerblom, Eva B. (Medicinal Chemistry, Pharmacia and Upjohn AB, Uppsala, SE-751 82, Swed.). Molecular Diversity, Volume Date 1998-1999, 4(1), 53-69 (English) 1999. CODEN: MODIF4. ISSN: 1381-1991. Publisher: Kluwer Academic Publishers.

AB Photolabile linkers are very useful in the generation of combinatorial libraries as they offer compd. cleavage under mild conditions directly into a solvent suitable for biol. testing. Photolabile linkers were developed which allow coupling of building blocks with a carboxy, amino, hydroxy and sulfonyl group. Photolytic cleavage of these building blocks will give libraries with carboxy, amido, methylamido, amino, ureido, hydroxy, aminocarbonyloxy and aminosulfonyl terminal groups. Coupling conditions for these reactions were elucidated and the photolytic cleavage reaction was studied.

IT **17324-90-2P**
(prepn. of)
RN 17324-90-2 HCA
CN Cyclohexanecarboxamide, 1-amino- (7CI, 9CI) (CA INDEX NAME)



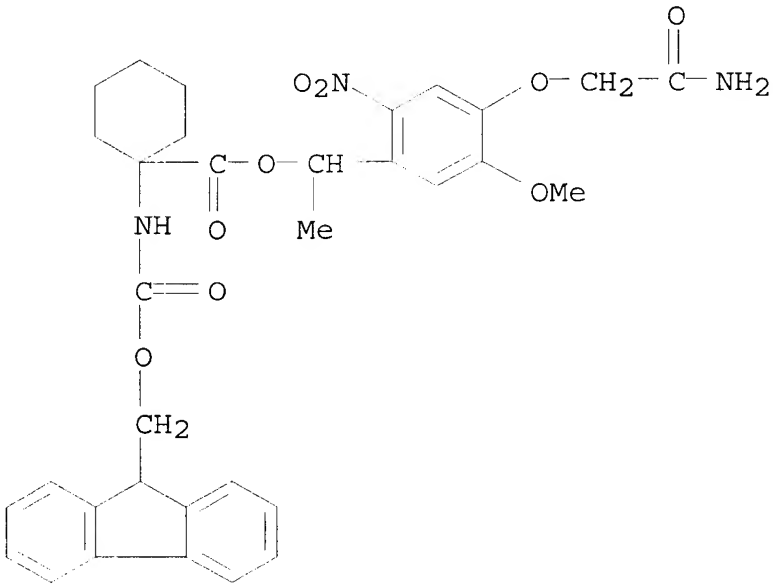
IT **162648-54-6**
(prepn. of photolabile linkers for **solid phase synthesis** and coupling of various building blocks and photolytic cleavage)
RN 162648-54-6 HCA
CN Cyclohexanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



IT **229028-27-7DP**, polymer-supported **229028-34-6DP**, polymer-supported
(prepn. of photolabile linkers for **solid phase synthesis** and coupling of various building blocks and photolytic cleavage)

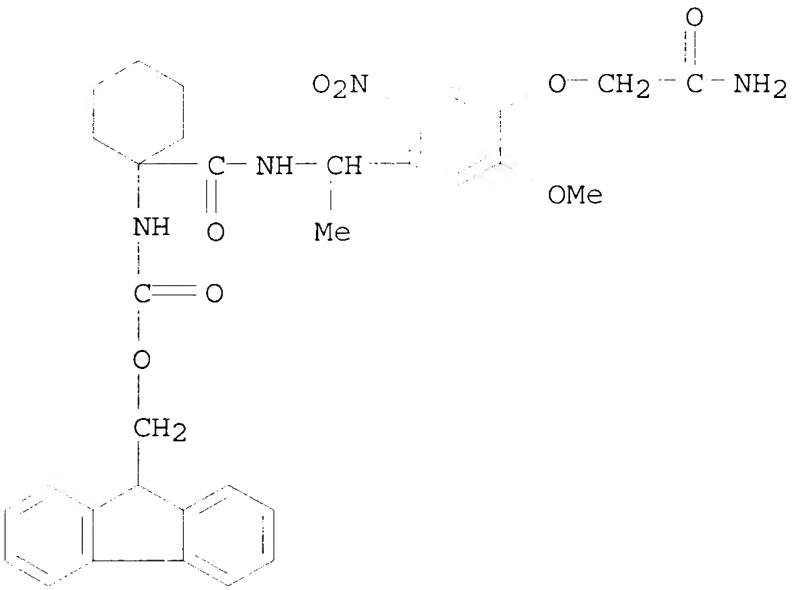
RN 229028-27-7 HCA

CN Cyclohexanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-, 1-[4-(2-amino-2-oxoethoxy)-5-methoxy-2-nitrophenyl]ethyl ester (9CI) (CA INDEX NAME)



RN 229028-34-6 HCA

CN Carbamic acid, [1-[[[1-[4-(2-amino-2-oxoethoxy)-5-methoxy-2-nitrophenyl]ethyl]amino]carbonyl]cyclohexyl]-, 9H-fluoren-9-ylmethyl ester (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)

ST photolabile linker **prepn solid phase synthesis**

IT **Solid phase synthesis**
(**prepn**. of photolabile linkers for **solid phase synthesis** and coupling of various building blocks and photolytic cleavage)

IT **17324-90-2P** 162576-07-0P 183990-60-5P 229028-57-3DP, polymer-supported 229028-67-5P 229028-68-6P 229028-69-7P 229028-70-0P 229028-71-1P 229028-72-2P 229028-73-3P
(prepn. of)

IT 78-81-9, Isobutylamine 98-74-8 103-90-2, 4-(Acetylamino)phenol 501-52-0, Benzenepropanoic acid 541-41-3, Carbonochloridic acid ethyl ester 6269-89-2, 1-(4-Nitrophenyl)piperazine 7693-46-1, Carbonochloridic acid 4-nitrophenyl ester 13734-41-3 24954-67-4, 4-Nitrobenzeneethanamine 45159-34-0 83435-58-9 130972-89-3, 4-(BOC-aminomethyl)-2-methoxyphenol 150736-72-4
162648-54-6 181232-20-2, TentaGel S-NH2 185116-43-2 187089-27-6 212007-03-9, 4-(1-Bromoethyl)-2-methoxy-5-nitrophenoxy]acetic acid 229028-23-3 229028-31-3D, polymer-supported 229028-32-4D, polymer-supported 229028-38-0 229028-39-1, 2-(BOCamino)butyl p-nitrophenyl carbonate 229028-41-5D, polymer-supported 229028-42-6D, polymer-supported 229028-43-7D, polymer-supported 229028-44-8 229028-46-0 229028-56-2D, polymer-supported 229028-61-9 229028-62-0
(prepn. of photolabile linkers for **solid phase synthesis** and coupling of various building blocks and

photolytic cleavage)
IT 770-39-8DP, polymer-supported 130972-89-3DP, polymer-supported
229028-21-1DP, 2-[4-(1-Bromoethyl)-2-methoxy-5-
nitrophenoxy]acetamide, polymer-supported 229028-22-2DP,
2-[4-(1-Hydroxyethyl)-2-methoxy-5-nitrophenoxy]acetamide,
polymer-supported 229028-30-2P
(prepn. of photolabile linkers for **solid phase synthesis** and coupling of various building blocks and photolytic cleavage)
IT 229028-24-4DP, polymer-supported 229028-25-5DP, polymer-supported
229028-26-6DP, polymer-supported **229028-27-7DP**,
polymer-supported 229028-28-8DP, polymer-supported
229028-29-9DP, polymer-supported 229028-33-5DP, polymer-supported
229028-34-6DP, polymer-supported 229028-35-7DP,
polymer-supported 229028-36-8DP, polymer-supported
229028-37-9DP, polymer-supported 229028-40-4DP, polymer-supported
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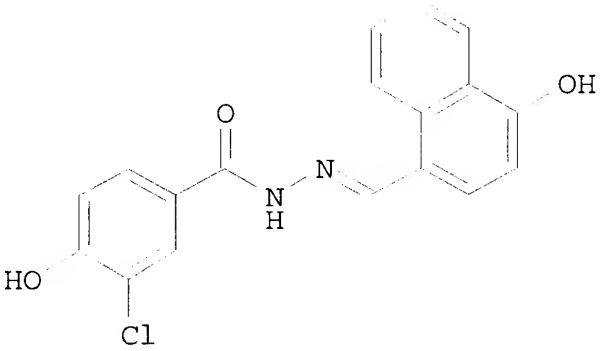
229028-49-3DP, polymer-supported 229028-50-6DP, polymer-supported
229028-51-7DP, polymer-supported 229028-52-8DP, polymer-supported
229028-53-9DP, polymer-supported 229028-54-0DP, polymer-supported
229028-55-1DP, polymer-supported 229028-58-4DP, polymer-supported
229028-59-5DP, polymer-supported 229028-60-8DP, polymer-supported
229028-63-1DP, polymer-supported 229028-64-2DP, polymer-supported
229028-65-3DP, polymer-supported 229028-66-4DP, polymer-supported
(prepn. of photolabile linkers for **solid phase synthesis** and coupling of various building blocks and photolytic cleavage)

L44 ANSWER 24 OF 36 HCA COPYRIGHT 2003 ACS
130:110061 Preparation of aroylhydrazones as glucagon antagonists/inverse agonists.. Gonzales, Javier; Sams, Christian; Teng, Min; Ling, Anthony; Gregor, Vlad; Hong, Yufeng; Kiel, Dan; Kuki, Atsuo; Shi, Shenghua; Naerum, Lars; Madsen, Peter; Lau, Jesper; Plewe, Michael Bruno; Feng, Jun; Johnson, Michael David; Teston, Kimberly Ann; Sidelmann, Ulla Grove; Knudsen, Lotte Bjerre (Novo Nordisk A/S, Den.; Alanex Corporation; et al.). PCT Int. Appl. WO 9901423 A1 19990114, 551 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-DK287 19980701. PRIORITY: US 1997-886785 19970701.
GI



I

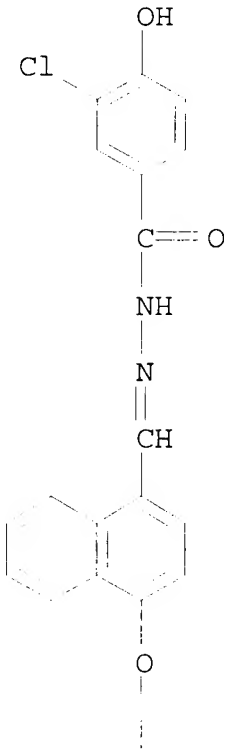
AB AXNR3NR1CR3R4(CH2)nBKmD [R1, R2= H, alkyl; R1R2 = bond; R3, R4 = H, alkyl; n = 0-3; m = 0, 1; X = CO, CS, C:NR5, SO2; R5 = H, alkyl, aralkyl, OR6; R6 = H, alkyl, aryl, aralkyl; A = (substituted) Ph, pyridyl, pyrimidinyl, naphthyl, indolyl, benzotriazolyl, imidazolyl, triazolyl, benzothiazolyl, pyrazolyl, isoxazolyl, oxazolyl, thienyl, furyl, etc.; B = bond, specified (substituted) (hetero)arylene, benzo(hetero)arylene, etc.; K = Le(CH2)b(CR3aR3b)p(CH2)aMf(CH2)c(CR4aCR4b)q(CH2)d; R3a, R3b, R4a, R4b = H, halo, cyano, CF3, OCF3, OCH2CF3, NO2, alkyl, aryl, aryalkyl, SCF3, CHF2, OSO2CF3, etc.; R3aR3b, R4aR4b, or R3aR4b = (CH2)i; i = 1-4; a, b, c, d = 0-4; e, f, p = 0, 1; q = 0-2; D = H, specified (substituted) (hetero)aryl, benzo(hetero)aryl], were prepd. as antidiabetics (no data). Thus, 3-chloro-4-hydroxybenzoic acid hydrazide (prepn. given) and 4-hydroxy-1-naphthaldehyde were stirred overnight in Me2SO/HOAc to give title compd. (I).

IT **219681-80-8P**
(prepn. of aroylhydrazones as glucagon antagonists/inverse agonists)

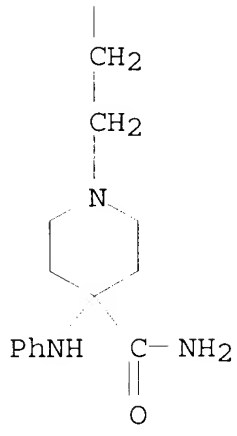
RN 219681-80-8 HCA

CN Benzoic acid, 3-chloro-4-hydroxy-, [[4-[2-[4-(aminocarbonyl)-4-(phenylamino)-1-piperidinyl]ethoxy]-1-naphthalenyl]methylene]hydrazide (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



IC ICM C07C243-18
ICS C07D209-04; A61K031-15; A61K031-40
CC 25-22 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 1, 27

ST aroylhydrazone prepn glucagon antagonist inverse agonist; antidiabetic aroylhydrazone prepn; hyperglycemia treatment aroylhydrazone; **solid phase synthesis** aroylhydrazone glucagon antagonist inverse agonist; combinatorial synthesis aroylhydrazone glucagon antagonist inverse agonist

IT Antidiabetic agents
Combinatorial library
Solid phase synthesis
(**prepn**. of aroylhydrazones as glucagon antagonists/inverse agonists)

IT 42596-21-4P 51771-18-7P 198897-90-4P 219680-20-3P
219680-23-6P 219680-26-9P 219680-29-2P 219680-31-6P
219680-33-8P 219680-35-0P 219680-36-1P 219680-37-2P
219680-38-3P 219680-39-4P 219680-41-8P 219680-42-9P
219680-43-0P 219680-44-1P 219680-45-2P 219680-48-5P
219680-50-9P 219680-52-1P 219680-54-3P 219680-56-5P
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219680-84-9P 219680-86-1P 219680-88-3P 219680-90-7P
219680-92-9P 219680-93-0P 219680-94-1P 219680-95-2P
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219683-08-6P 219683-09-7P 219683-10-0P 219683-11-1P
219683-12-2P
(prepn. of aroylhydrazones as glucagon antagonists/inverse agonists)

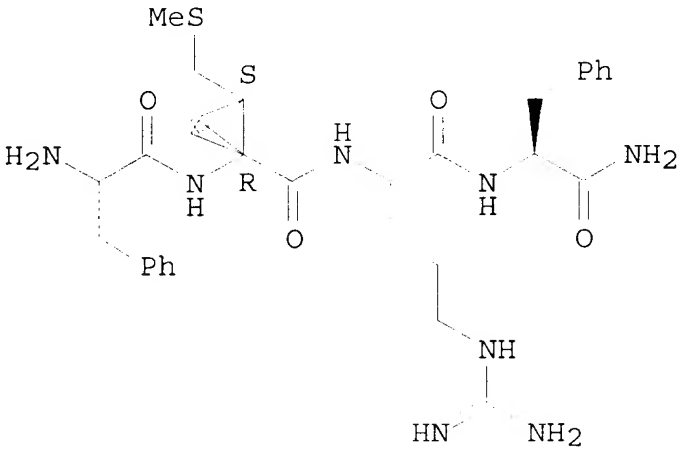
IT 65-49-6, 4-Aminosalicylic acid 75-33-2, Isopropyl mercaptan 78-81-9, Isobutylamine 79-04-9, Chloroacetyl chloride 91-21-4, 1,2,3,4-Tetrahydroisoquinoline 96-32-2, Methyl bromoacetate 99-76-3, Methyl 4-hydroxybenzoate 100-36-7, N,N-Diethylethylenediamine 100-52-7, Benzaldehyde, reactions 105-36-2, Ethyl bromoacetate 106-93-4, 1,2-Dibromoethane 106-95-6, Allyl bromide, reactions 107-04-0, 1-Bromo-2-chloroethane 109-89-7, reactions 121-33-5, Vanillin 134-96-3, Syringaldehyde 140-88-5 350-29-8, 3-Fluoro-4-hydroxybenzoic acid 487-89-8, 3-Formylindole 536-25-4, Methyl 3-amino-4-hydroxybenzoate 605-70-9, Naphthalene-1,4-dicarboxylic acid 621-59-0, 3-Hydroxy-4-methoxybenzaldehyde 659-28-9, 4-Trifluoromethoxybenzaldehyde 867-13-0, Triethyl phosphonoacetate 1013-25-8, 4-(2,5-Dimethylphenyl)piperazine 1192-30-9, 2-(Bromomethyl)tetrahydrofuran 2051-18-5, 4-Isopropylbenzyl chloride 2233-18-3, 3,5-Dimethyl-4-hydroxybenzaldehyde 2457-76-3, 4-Amino-2-chlorobenzoic acid 2486-69-3, 4-Amino-3-methoxybenzoic acid 2759-28-6, 1-Benzylpiperazine 2840-26-8, 3-Amino-4-methoxybenzoic acid 2973-76-4, 5-Bromovanillin 2973-77-5, 3,5-Dibromo-4-hydroxybenzaldehyde 3132-64-7, 2,3-Epoxypropyl bromide 3179-31-5, 1,2,4-Triazole-3-thiol 3300-51-4, 4-Trifluoromethylbenzylamine 3466-80-6, 2-Phenylpiperidine 3964-57-6, Methyl 3-chloro-4-hydroxybenzoate 4488-40-8, 4-Methyl-1-naphthoic acid 5438-36-8, 5-Iodovanillin 7770-45-8 14311-34-3 15761-39-4 15861-24-2, 5-Cyanoindole 18278-34-7, 4-Hydroxy-2-methoxybenzaldehyde 19463-48-0, 3-Chloro-4-hydroxy-5-methoxybenzaldehyde 22118-09-8, Bromoacetyl chloride 24985-85-1, Ethyl 5-hydroxyindole-2-carboxylate 25319-94-2 27492-84-8, Methyl 4-amino-2-methoxybenzoate 32247-96-4, 3,5-Bis(trifluoromethyl)benzyl bromide 38212-33-8,

1-(4-Chlorophenyl)piperazine 39634-98-5 39634-98-5D, 3-Chloro-4-hydroxybenzoic acid hydrazide, **resin-bound** 39635-02-4D, 3-Fluoro-4-hydroxybenzoic acid hydrazide, **resin-bound** 57988-58-6 68634-82-2 69833-14-3 93919-56-3 114715-38-7, (S)-1-Benzyl-3-aminopyrrolidine 114715-39-8, (R)-1-Benzyl-3-aminopyrrolidine 126162-38-7 219685-69-5 219685-70-8 219685-71-9 219685-73-1 219685-74-2D, **resin-bound** 219685-75-3
(prepn. of aroylhydrazones as glucagon antagonists/inverse agonists)

L44 ANSWER 25 OF 36 HCA COPYRIGHT 2003 ACS

126:8665 On the Conformational Bias of F(2(R),3(S)-cyclo-M)RFa Induced by the cis-2,3-Methanomethionine Residue. Burgess, Kevin; Ke, Chun-Yen (Department of Chemistry, Texas A + M University, College Station, TX, 77843-3255, USA). Journal of Organic Chemistry, 61(24), 8627-8631 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

GI



I

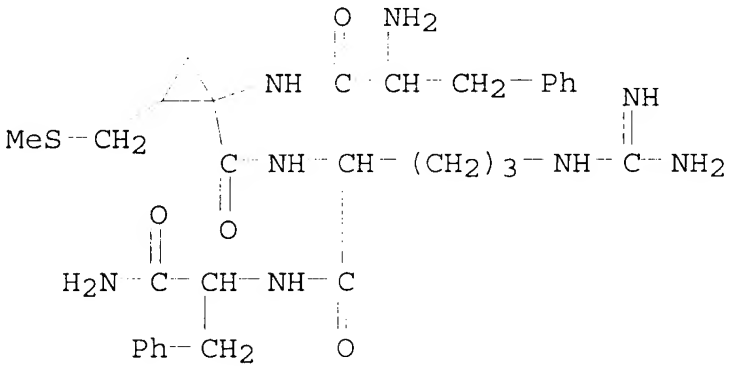
AB The objective of this work was to study conformational biases attributable to a cis-2,3-methanomethionine isomer substituted in a model sequence, FMRFa, and to compare them with previous studies of trans-2,3-methanomethionine stereoisomers in the same environment. Consequently, F(2(R),3(S)-cyclo-M)RFa (I) was **prepd.** via **solid phase synthesis** and solns. of this material were examd. by NMR and CD spectroscopies. These spectral studies were complemented by mol. simulations. These computational studies indicated .gamma.- and .beta.-turn structures were favored; however, the exptl. data are consistent with only the .gamma.-turn structure. Overall, this work and previous research indicates that both cis- and trans-2,3-methanomethionine stereoisomers tend to impart a conformational preference for .gamma.-turns when

substituted for methionine in FMRFa. It is proposed that this phenomenon is indirectly due to widening of the N-C.alpha.-CO bond angle by the cyclopropane and might therefore be obsd. for 2,3-methanomethionine residues in other sequences.

IT **147126-89-4P**
(conformational bias of peptide induced by methanomethionine residue)

RN 147126-89-4 HCA

CN L-Phenylalaninamide, L-phenylalanyl-cis-2-[(methylthio)methyl]-(R)-1-aminocyclopropanecarbonyl-L-arginyl- (9CI) (CA INDEX NAME)

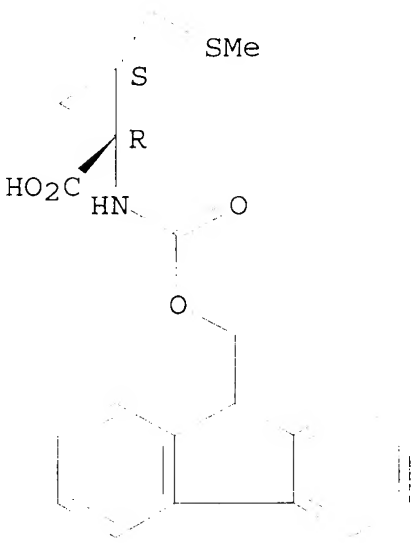


IT **183902-49-0**
(conformational bias of peptide induced by methanomethionine residue)

RN 183902-49-0 HCA

CN Cyclopropanecarboxylic acid, 1-[[(9H-fluoren-9-ylmethoxy)carbonyl]amino]-2-[(methylthio)methyl]-, (1R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22

IT **147126-89-4P**
(conformational bias of peptide induced by methanomethionine residue)

IT 35661-40-6 98930-01-9 130858-97-8 **183902-49-0**
(conformational bias of peptide induced by methanomethionine residue)

L44 ANSWER 26 OF 36 HCA COPYRIGHT 2003 ACS

124:30439 Preparation of opioid peptides as analgesics.. Brown, William; Dimaio, John; Schiller, Peter; Martel, Rene (Astra AB, Swed.). PCT Int. Appl. WO 9522557 A1 19950824, 48 pp. DESIGNATED STATES: W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, UG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1995-SE158 19950215. PRIORITY: GB 1994-3263 19940221; GB 1994-8179 19940425; SE 1994-1519 19940503.

AB X-A1-A2-A3-Q-A4-NYZ [X = H, alkyl; Y, Z = H, alkyl, aralkyl; A1 = Tyr, 2',6'-dimethyltyrosyl, analog thereof; A2 = (R)-amino acid residue; A3, A4 = arom. amino acid residue; Q = amide bond, amide bond mimetic; with provisos], were prepd. Thus, H-Tyr-D-Ala-Phe-Phe-NH2, **prepd.** by **solid phase synthesis** on Rink resin, showed an ED50 = 1.4 mg/kg for inhibition of phenylbenzoquinone-induced writhing in mice. The peptides of the present invention act substantially on peripheral .mu.-opioid receptors,substantially avoiding side effects normally assocd. with central analgesic action.

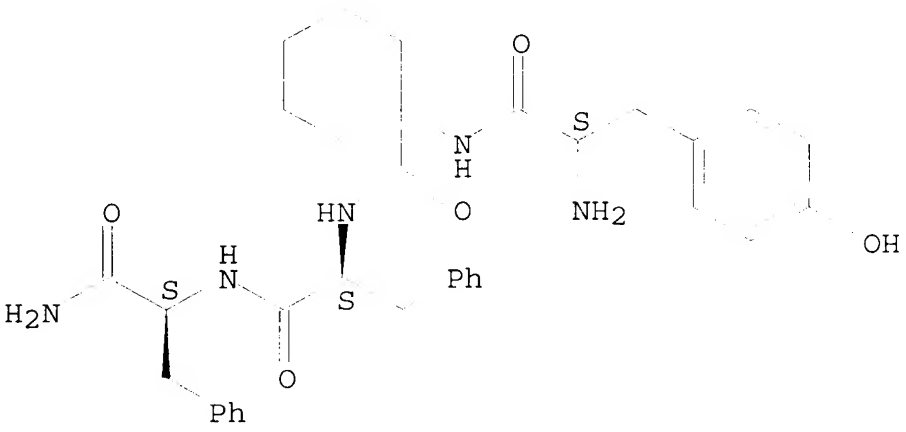
IT **171807-56-0P 171807-57-1P**

(prepn. of opioid peptides as analgesics)

RN 171807-56-0 HCA

CN L-Phenylalaninamide, L-tyrosyl-1-aminocyclohexanecarbonyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

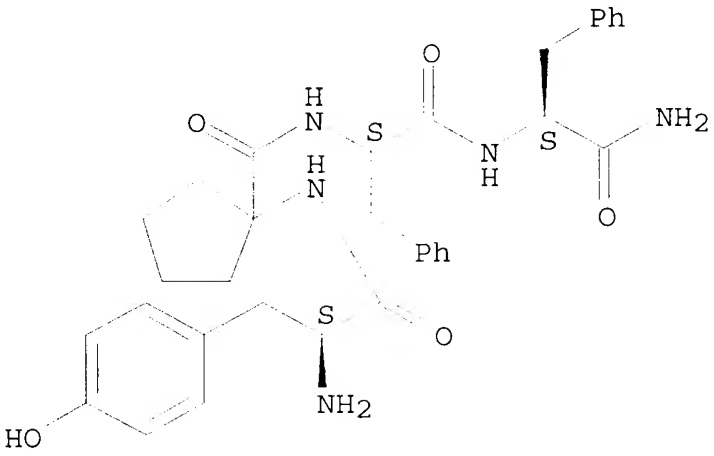
Absolute stereochemistry.



RN 171807-57-1 HCA

CN L-Phenylalaninamide, L-tyrosyl-1-aminocyclopentanecarbonyl-L-phenylalanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07K005-107

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1

IT 118476-87-2P 124777-74-8P 124777-75-9P 124777-76-0P
124777-77-1P 124777-78-2P 141801-26-5P 147658-92-2P
171807-33-3P 171807-34-4P 171807-35-5P 171807-36-6P
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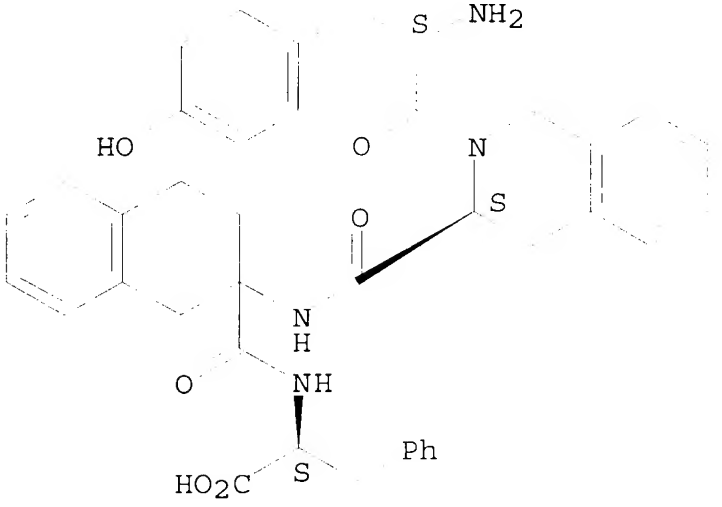
171807-94-6P 171807-95-7P 171807-97-9P
(prepn. of opioid peptides as analgesics)

L44 ANSWER 27 OF 36 HCA COPYRIGHT 2003 ACS
122:188168 Preparation of peptides as .delta. opioid antagonists..
Schiller, Peter (Aktiebolaget Astra, Swed.). PCT Int. Appl. WO 9415959 A1 19940721, 36 pp. DESIGNATED STATES: W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, UZ, VN; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1993-SE1090 19931220. PRIORITY: SE 1993-12 19930105.
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

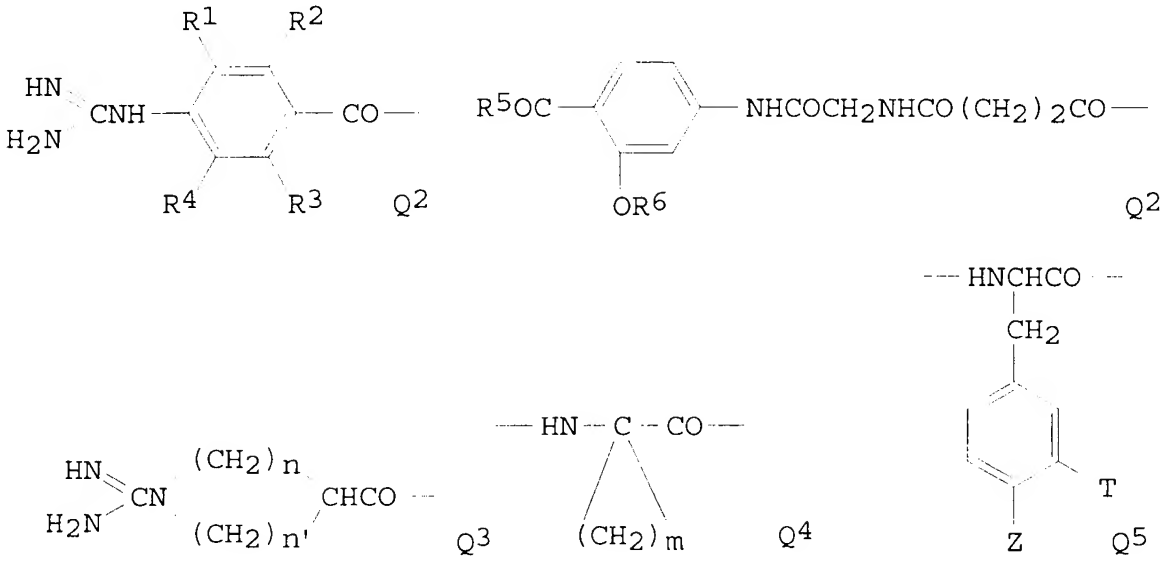
AB Title compds. [I; R1 = H, Me(CH2)n, PhCH2CH2, cyclopropylmethyl, allyl, H-Arg; R2 = H, Me(CH2)n, cyclopropylmethyl, allyl, etc.; n = 0-12; R3-R6 = H, or R4, R5 both = H and R3, R6 both = lower alkyl, or R3, R5, R6all = H and R4 = F, Cl, Br, OH, NH2, NO2; R7 = CO, CH2; R8= H, lower alkyl; R9= Q1-Q7; m = 0-2; R10 = H, F, Cl, Br, iodo; R11 = OH, NH2, Q8, Q9; R12 = H, NO2, F, Cl, Br, iodo; m = 0-2; R13, R14 = CO2H, CONH2, CH2OH, amino acid or peptide segment; with the exceptions of compds. where R1, R2, R3, R4, R5, R6, R8 all = H, R7 = CO, R9 = PhCH2CH, and R11 = Phe-OH, Phe-NH2, OH, NH2], were prepd. Thus, H-Tyr-Tic-Hfe-Phe-OH (Tic = 1,2,3,4-tetrahydroisoquinoline-3-carboxylate; Hfe = homophenylalanyl), was **prepd.** by **solid phase synthesis.** I antagonized [Leu5] enkephalin in mouse vas deferens with Ke = 0.169-43.9 nM.
IT **161669-10-9**
(peptides as .delta. opioid antagonists)
RN 161669-10-9 HCA
CN L-Phenylalanine, L-tyrosyl-L-1,2,3,4-tetrahydro-3-isoquinolinecarbonyl-1,2,3,4-tetrahydro-2-amino-2-naphthalenecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07K005-10
ICS C07C005-08; C07K007-12; C07K005-02; A61K037-02
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1
IT 143293-99-6 146369-65-5 147685-18-5 147731-91-7 147731-92-8
156219-35-1 156219-36-2 156219-37-3 156248-24-7 159992-07-1
160115-86-6 160115-87-7 160429-67-4 160429-68-5 161668-96-8
161668-97-9 161668-98-0 161668-99-1 161669-00-7 161669-01-8
161669-02-9 161669-03-0 161669-04-1 161669-05-2 161669-06-3
161669-07-4 161669-08-5 161669-09-6 **161669-10-9**
161669-11-0 161669-12-1 161669-13-2 161669-14-3 161754-62-7
(peptides as .delta. opioid antagonists)
IT 2577-40-4D, **resin bound** 13734-34-4D,
resin bound 20866-48-2 78879-20-6, BOC-Tic-OH
100564-78-1
(prepn. of peptides as .delta. opioid antagonists)
IT 145525-27-5P 156219-35-1DP, **resin bound**
160941-21-9P
(prepn. of peptides as .delta. opioid antagonists)

L44 ANSWER 28 OF 36 HCA COPYRIGHT 2003 ACS
120:218550 Preparation of hirudin derivatives as anticoagulants.
Fauchere, Jean Luc; Thurieau, Christophe; Verbeuren, Tony; Paladino, Joseph (Adir et Cie., Fr.). Eur. Pat. Appl. EP 552999 A1 19930728, 27 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE. (French). CODEN: EPXXDW. APPLICATION: EP 1993-400051 19930113. PRIORITY: FR 1992-340 19920115.
GI



AB X-A1-A2-A3-A4-A5-A6-A7-A8-A9-A10-Y [I; X = H2N-C(:NH)-NH(CH2)p-CO, Q1, Q2, Q3; 1.ltoreq.p.ltoreq.5; n, n' = 1-6 integer; R1-R4 = H, alkyl, halo, etc.; R5 = alkyl, OH; R6 = H, acyl; A1 = bond, a peptide resulting optionally contg. Q4; m = 2-7 integer; A2 = bond, Phe, Tyr, Ile, etc.; A3 = bond, Glu, Asp, Tyr, Q4; A4 = bond, Glu, Asp, Pro, Q4, 2-azabicyclo[2.2.2]octane-3-carbonyl (Abo), etc.; A5 = bond, Ile, Nva, Phe, etc.; A6 = Pro, Ile, Nva, Phe, Orn, Abo, etc.; A7 = Glu, Asp, Q4; A8 = Glu, Asp, 2,3-diaminopropionic acid residue, Q4, etc.; A9 = Q5; Z, T = H, OPO3H2, PO3H2, CH2-CO2H, OH; A10 = bond, Leu, Val, etc.; Y = OH, alkoxy, etc.; with provisos] are prepd. and their anticoagulant activity is evaluated. Thus, p-H2N-C(:NH)-NH-C6H4-CO-Gly-Asp-Phe-Glu-Abo-Ile-Pro-Glu-Glu-Tyr(mPO3H2)-Leu-glu-OH.CF3CO2H (II) was **prepd.** by the **solid-phase** method from **resin-bound** Fmoc-glu(OtBu)-OH via sequential peptide coupling with Fmoc-Leu-OH, Fmoc-Tyr[(pOBzl),(mPO3Me2)]-OH, Fmoc-Glu(OtBu)-OH, Fmoc-Glu(OtBu)-OH, Fmoc-Pro-OH, Fmoc-Ile-OH, Fmoc-Abo-OH, Fmoc-Glu(OtBu)-OH, Fmoc-Phe-OH, Fmoc-Asp(OtBu)-OH, and Fmoc-Gly-OH. According to an in vivo study using rats, I (not specified) prolonged the coagulation time .ltoreq.5000% compared with the control and .gtoreq.30000% compared with hirudin. A soln. for injection and a tablets contg. II were formulated.

IT **154038-77-4P**
(prepn. of, as anticoagulant)

RN 154038-77-4 HCA

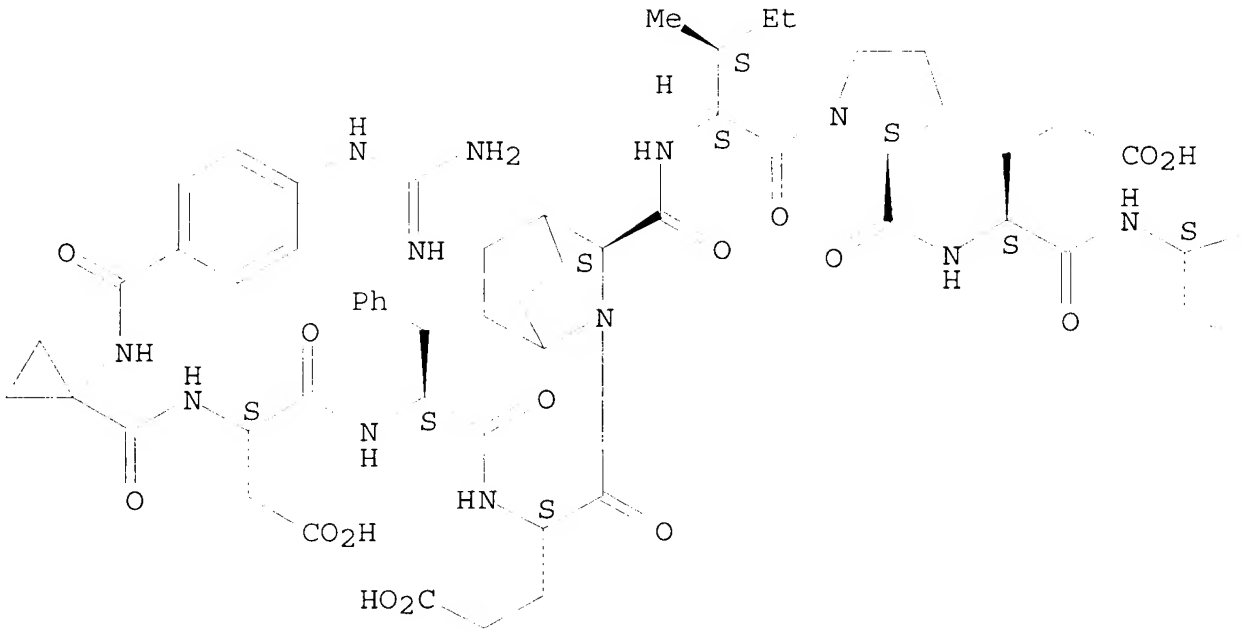
CN D-Glutamic acid, N-[[1-[[4-[(aminoiminomethyl)amino]benzoyl]amino]cyclopropyl]carbonyl]-L-.alpha.-aspartyl-L-phenylalanyl-L-.alpha.-glutamyl-L-2-azabicyclo[2.2.2]octane-3-carbonyl-L-isoleucyl-L-prolyl-L-.alpha.-glutamyl-L-.alpha.-glutamyl-O-phosphono-L-tyrosyl-L-leucyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

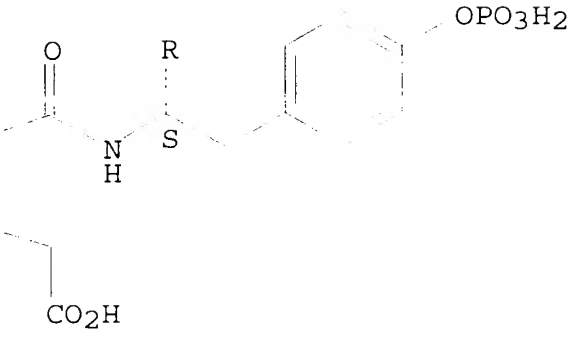
CRN 154038-76-3
CMF C79 H106 N15 O28 P

Absolute stereochemistry.

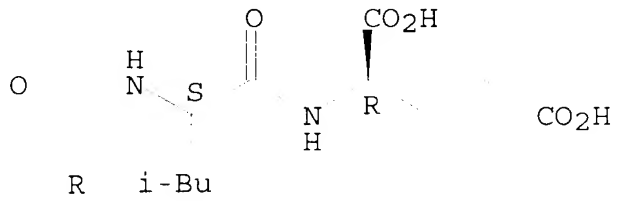
PAGE 1-A



PAGE 1-B

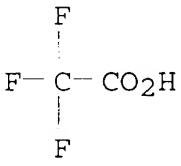


PAGE 2-A



CM 2

CRN 76-05-1
CMF C2 H F3 O2



IC ICM C07K007-06
ICS C07K007-08; A61K037-02
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 63
IT **154038-77-4P** 154038-79-6P 154038-81-0P 154099-00-0P
(prepn. of, as anticoagulant)
IT 29022-11-5, Fmoc-Gly-OH 35661-40-6 35661-60-0 71989-14-5
71989-23-6 71989-31-6 104091-08-9 104091-08-9D, **resin-bound** 135544-65-9 144976-83-0 153887-03-7
154038-82-1D, **resin-bound**
(reaction of, in prepn. of anticoagulants)

L44 ANSWER 29 OF 36 HCA COPYRIGHT 2003 ACS
120:49085 Technetium-99m labeled peptides for imaging inflammation. Dean, Richard T.; Lees, Robert S.; Buttram, Scott; Lister-James, John (Diatech, Inc., USA). PCT Int. Appl. WO 9317719 A1 19930916, 40 pp. DESIGNATED STATES: W: AU, CA, JP, KR, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1993-US2320 19930312. PRIORITY: US 1992-851074 19920313.
AB Scintig. agents for imaging inflammation sites comprise a peptide covalently bound to 99mTc. The peptides are, e.g., Cp(aa)Cp (Cp = protected cysteine; aa = amino acid) or ACZB(CR1R2)nX (A = H, CO2H, CONH2, R4, peptidyl NHOC, CO2 peptidyl; B, X = H, SH, NHR3, NR3 peptidyl, R4; Z = H, R4; R1-4 = H, alkyl; n = 0, 1, 2). The peptides bind specifically to leukocytes, preferably neutrophils. The peptides were **prepd**. by **solid-phase**

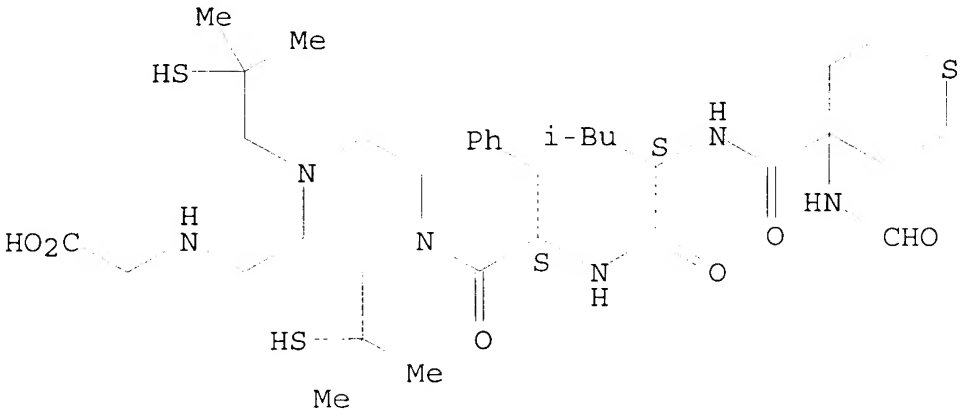
synthesis, as usual.

IT **152175-02-5D**, technetium-99m-labeled complexes
(scintigraphic imaging agents, for inflammation diagnosis)

RN 152175-02-5 HCA

CN L-Phenylalaninamide, N-[[4-(formylamino)tetrahydro-2H-thiopyran-4-yl]carbonyl]-L-leucyl-N-[2-[[2-[(carboxymethyl)amino]ethyl](2-mercapto-2-methylpropyl)amino]ethyl]-N-(2-mercapto-2-methylpropyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K049-02
ICS A61K043-00

CC 8-9 (Radiation Biochemistry)

IT 152174-83-9D, technetium-99m-labeled complexes 152174-84-0D,
technetium-99m-labeled complexes 152174-85-1D,
technetium-99m-labeled complexes 152174-86-2D,
technetium-99m-labeled complexes 152174-87-3D,
technetium-99m-labeled complexes 152174-88-4D,
technetium-99m-labeled complexes 152174-89-5D,
technetium-99m-labeled complexes 152174-90-8D,
technetium-99m-labeled complexes 152174-91-9D,
technetium-99m-labeled complexes 152174-92-0D,
technetium-99m-labeled complexes 152174-93-1D,
technetium-99m-labeled complexes 152174-94-2D,
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technetium-99m-labeled complexes 152174-98-6D,
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technetium-99m-labeled complexes **152175-02-5D**,
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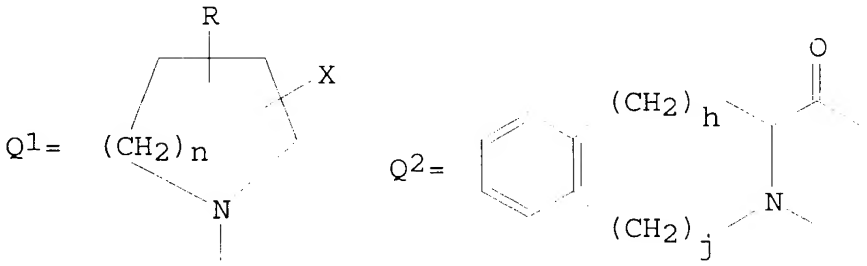
technetium-99m-labeled complexes 152206-07-0D,
technetium-99m-labeled complexes 152206-08-1D,
technetium-99m-labeled complexes
(scintigraphic imaging agents, for inflammation diagnosis)

L44 ANSWER 30 OF 36 HCA COPYRIGHT 2003 ACS
118:102472 Preparation of hexa- and heptapeptide anaphylatoxin-receptor ligands. Wiedeman, Paul E.; Kawai, Megumi; Luly, Jay R.; Or, Yat Sun; Wagner, Rolf (Abbott Laboratories, USA). PCT Int. Appl. WO 9211858 A1 19920723, 161 pp. DESIGNATED STATES: W: CA, JP; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1991-US9319 19911210. PRIORITY: US 1990-634641 19901227.

GI



AB A-B-D-E-G-J-L-M-Q [A = R1R2R3; B = R4R5R6, R35, R37; D = R7, R8, R9, R35; E = R10R11R12, R35; G = R13R14R15, R35; J = R16R17R18, R35; L = R19R20R21, R35; M = bond, R22R23R24, R35; Q = R25R26R27; R1 = aryl, alkyl, arylalkyl, H; R2 = O, (substituted) CH2; R1R2 = H, aryl; R1R2R3 = H, alkyl, aralkyl, alkenyl, protecting group; R3 = CO, CH2;

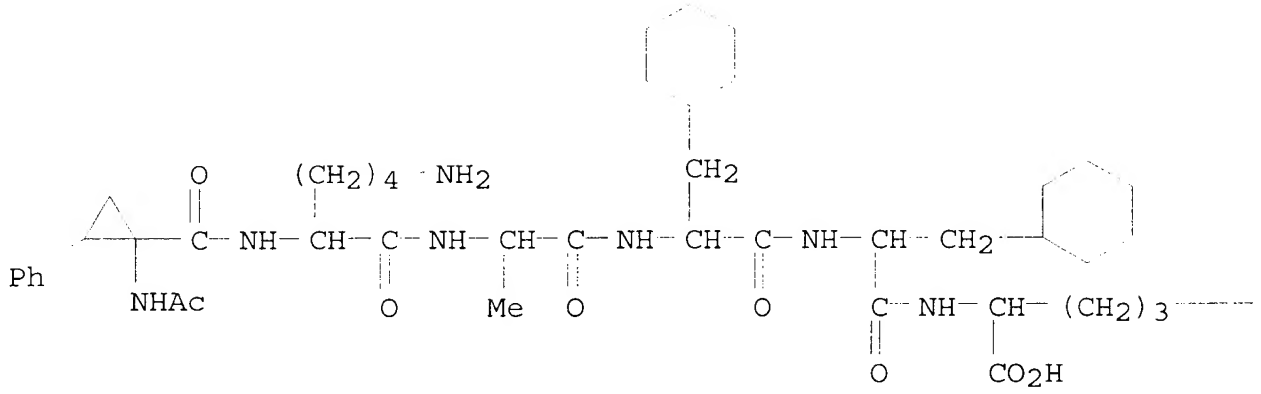
R4 = (substituted) NH; R5, R8, R14, R17 = (substituted) CH2, C:CH2, imino, cyclopropylene; R6, R9, R12, R15, R18, R21, R24 = CO; R7, R10, R13, R16, R19, R22 = NH; R20, R23 = (substituted) CH2, C:CH2, cyclopropylene; R25 = O, (substituted) NH; R26 = H, alkyl, oralkyl, (substituted) NH; R27 = H, aryl; R26R27 = H, alkyl, aralkyl; R35 = Q1; n = 0-2; X = CO; R = H, alkyl; R37 = h = 1; j = 0, 1], were prepd. Thus, H-Phe-Lys-Lys-Q3-Q4-D-Arg-OH [Q3 = (2R)-2-amino-3-cyclohexylpropanoyl, Q4 = (2S)-2-amino-3-cyclohexylpropanoyl] (**prepd.** by **solid phase** methods) bound to anaphylatoxin receptors with Ki = 0.011 .mu.m.

IT **144555-14-6P 144556-04-7P 144556-15-0P**
144556-24-1P 144556-32-1P 144571-18-6P
144596-25-8P 144596-40-7P 144607-90-9P
(prepn. of, as anaphylatoxin receptor ligand)

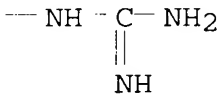
RN 144555-14-6 HCA

CN D-Arginine, N2-[N-[N-[N-[N2-[[1-(acetylamino)-2-phenylcyclopropyl]carbonyl]-L-lysyl]-L-alanyl]-3-cyclohexyl-D-alanyl]-3-cyclohexyl-L-alanyl]-, (1R-cis)- (9CI) (CA INDEX NAME)

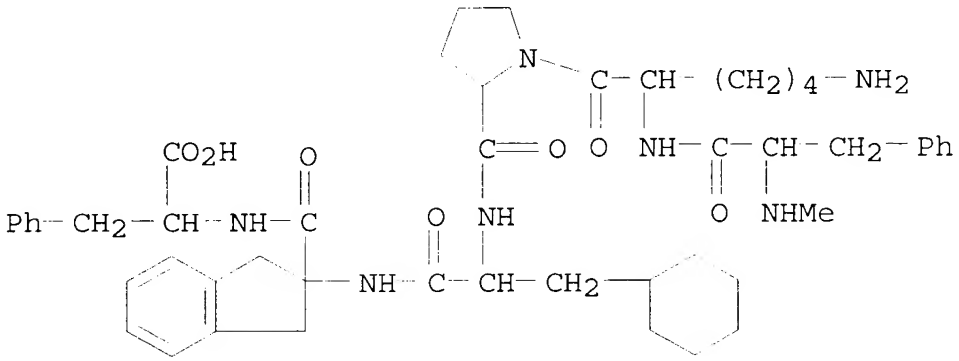
PAGE 1-A



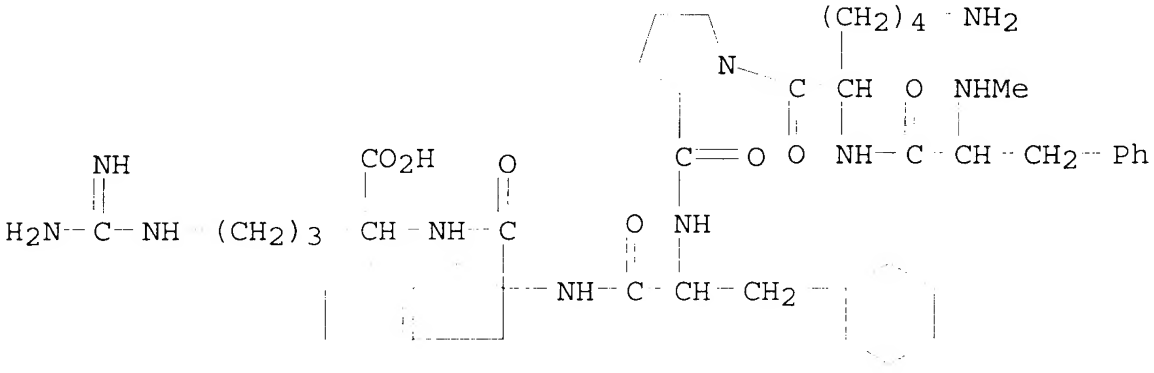
PAGE 1-B



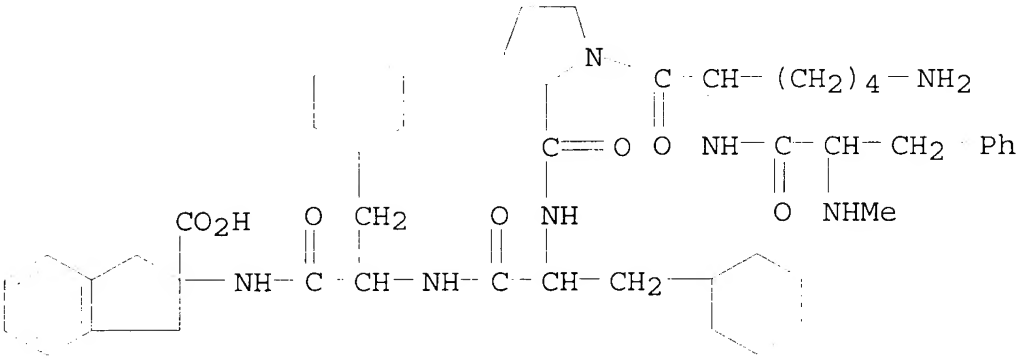
RN 144556-04-7 HCA
CN D-Phenylalanine, N-methyl-L-phenylalanyl-L-lysyl-L-prolyl-3-cyclohexyl-D-alanyl-2,3-dihydro-1H-indene-2-carbonyl- (9CI) (CA INDEX NAME)



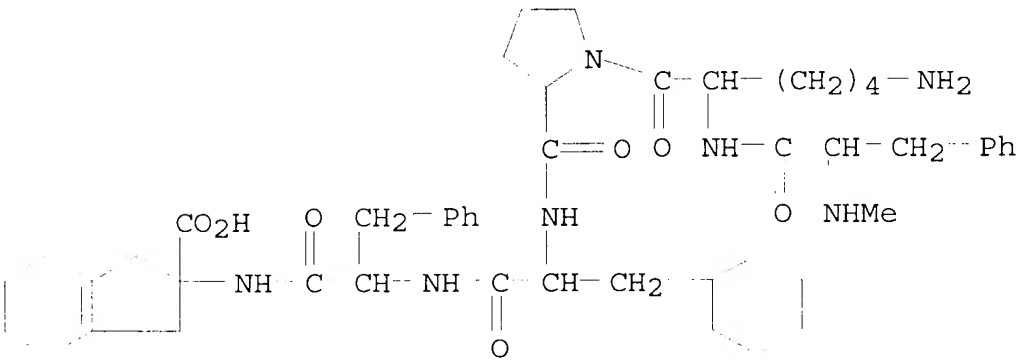
RN 144556-15-0 HCA
CN D-Arginine, N-methyl-L-phenylalanyl-L-lysyl-L-prolyl-3-cyclohexyl-D-alanyl-2,3-dihydro-2-amino-1H-indene-2-carbonyl- (9CI) (CA INDEX NAME)



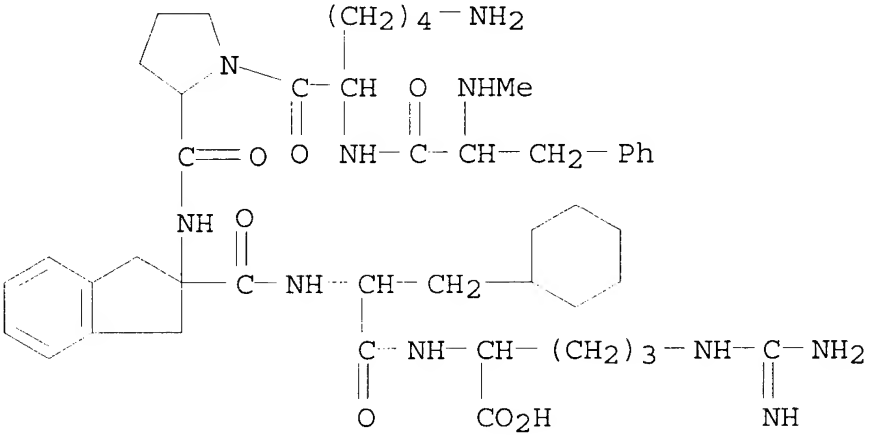
RN 144556-24-1 HCA
CN L-Alaninamide, N-methyl-L-phenylalanyl-L-lysyl-L-prolyl-3-cyclohexyl-D-alanyl-N-(2-carboxy-2,3-dihydro-1H-inden-2-yl)-3-cyclohexyl- (9CI) (CA INDEX NAME)



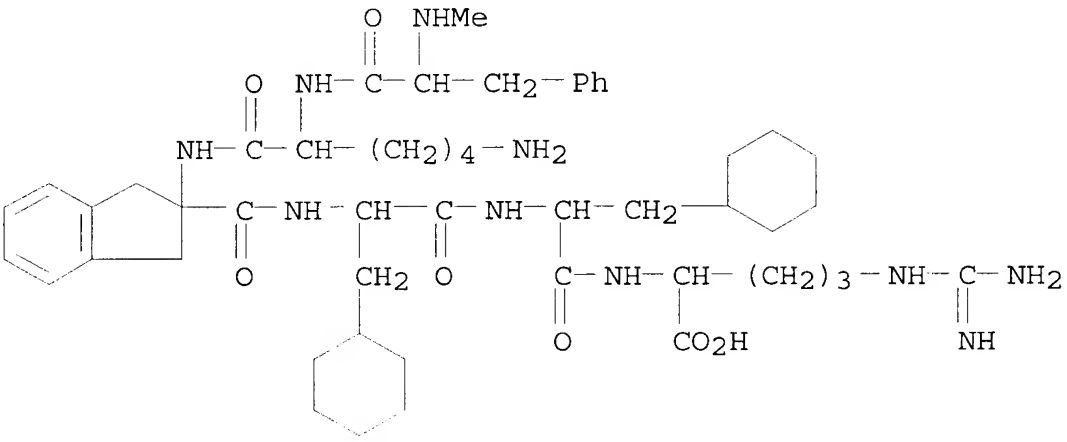
RN 144556-32-1 HCA
CN L-Phenylalaninamide, N-methyl-L-phenylalanyl-L-lysyl-L-prolyl-3-cyclohexyl-D-alanyl-N-(2-carboxy-2,3-dihydro-1H-inden-2-yl)- (9CI) (CA INDEX NAME)



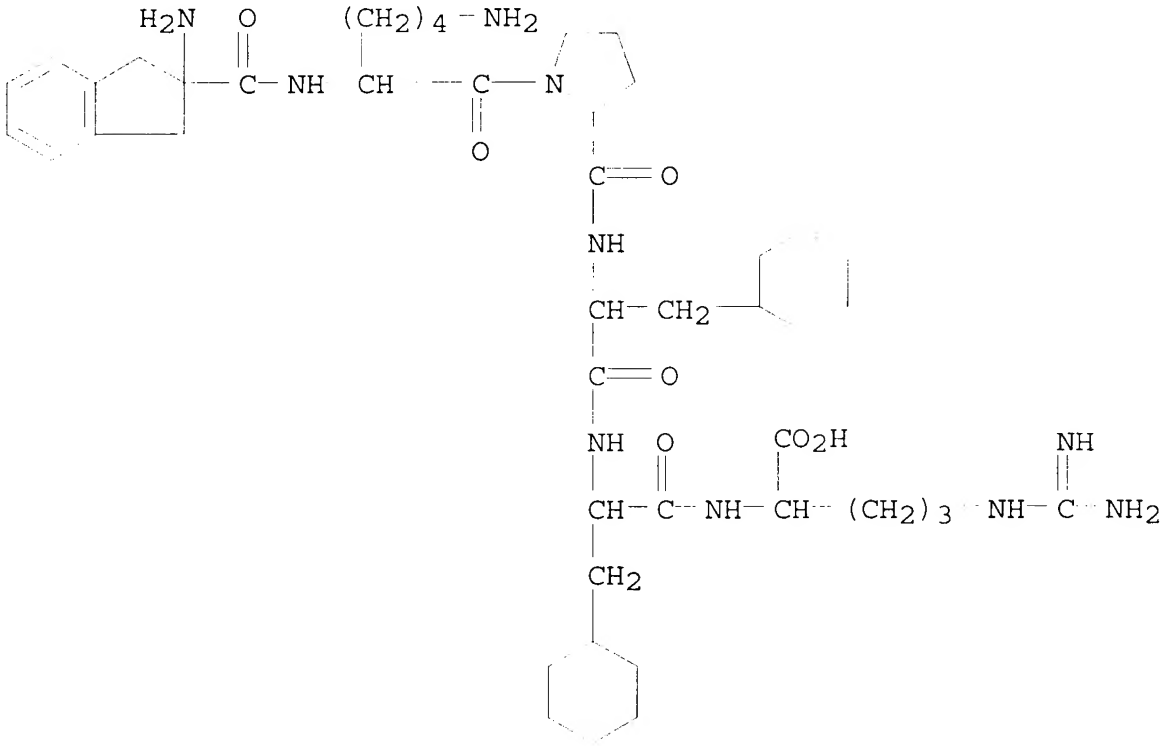
RN 144571-18-6 HCA
CN D-Arginine, N-methyl-L-phenylalanyl-L-lysyl-L-prolyl-2,3-dihydro-1H-indene-2-carbonyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)



RN 144596-25-8 HCA
CN D-Arginine, N-methyl-L-phenylalanyl-L-lysyl-2,3-dihydro-1H-indene-2-carbonyl-3-cyclohexyl-D-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

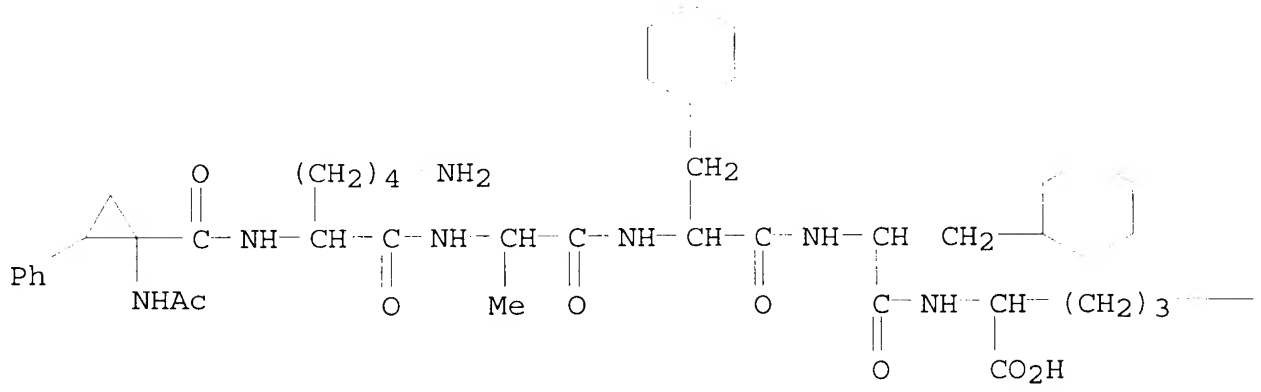


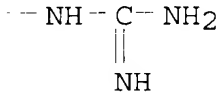
RN 144596-40-7 HCA
CN D-Arginine, N2-[N-[N-[1-[N2-[(2-amino-2,3-dihydro-1H-inden-2-yl)carbonyl]-L-lysyl]-L-prolyl]-3-cyclohexyl-D-alanyl]-3-cyclohexyl-L-alanyl]- (9CI) (CA INDEX NAME)



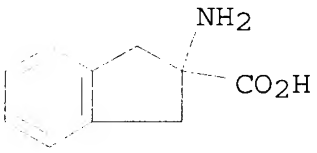
RN 144607-90-9 HCA
CN L-Arginine, N2-[N-[N-[N-[N2-[[1-(acetylamino)-2-phenylcyclopropyl]carbonyl]-L-lysyl]-L-alanyl]-3-cyclohexyl-D-alanyl]-3-cyclohexyl-L-alanyl]-, (1S-cis)- (9CI) (CA INDEX NAME)

PAGE 1-A



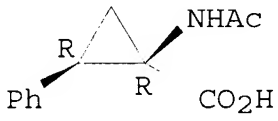


IT **27473-62-7P 144643-81-2P**
(prepn. of, as intermediate for peptide anaphylatoxin receptor ligand)
RN 27473-62-7 HCA
CN 1H-Indene-2-carboxylic acid, 2-amino-2,3-dihydro- (9CI) (CA INDEX NAME)



RN 144643-81-2 HCA
CN Cyclopropanecarboxylic acid, 1-(acetylamino)-2-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IC ICM A61K037-00
ICS A61K037-02; C07K005-00; C07K007-00; C07K015-00; C07K017-00
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1
IT 144554-77-8P 144554-78-9P 144554-79-0P 144554-80-3P
144554-81-4P 144554-82-5P 144554-83-6P 144554-84-7P
144554-85-8P 144554-86-9P 144554-87-0P 144554-88-1P
144554-89-2P 144554-90-5P 144554-91-6P 144554-92-7P
144554-93-8P 144554-94-9P 144554-95-0P 144554-96-1P
144554-97-2P 144554-98-3P 144554-99-4P 144555-00-0P

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144555-09-9P	144555-10-2P	144555-11-3P	144555-12-4P
144555-13-5P	**144555-14-6P**	144555-15-7P	144555-16-8P
144555-17-9P	144555-18-0P	144555-19-1P	144555-20-4P
144555-21-5P	144555-22-6P	144555-23-7P	144555-24-8P
144555-25-9P	144555-26-0P	144555-27-1P	144555-28-2P
144555-29-3P	144555-30-6P	144555-31-7P	144555-32-8P
144555-33-9P	144555-34-0P	144555-35-1P	144555-36-2P
144555-37-3P	144555-38-4P	144555-39-5P	144555-40-8P
144555-41-9P	144555-42-0P	144555-43-1P	144555-44-2P
144555-45-3P	144555-46-4P	144555-47-5P	144555-48-6P
144555-49-7P	144555-50-0P	144555-51-1P	144555-52-2P
144555-53-3P	144555-54-4P	144555-55-5P	144555-56-6P
144555-57-7P	144555-58-8P	144555-59-9P	144555-60-2P
144555-61-3P	144555-62-4P	144555-63-5P	144555-64-6P
144555-65-7P	144555-66-8P	144555-67-9P	144555-68-0P
144555-69-1P	144555-70-4P	144555-71-5P	144555-72-6P
144555-73-7P	144555-74-8P	144555-75-9P	144555-76-0P
144555-77-1P	144555-78-2P	144555-79-3P	144555-80-6P
144555-81-7P	144555-82-8P	144555-83-9P	144555-84-0P
144555-85-1P	144555-86-2P	144555-87-3P	144555-88-4P
144555-89-5P	144555-90-8P	144555-91-9P	144555-92-0P
144555-93-1P	144555-94-2P	144555-95-3P	144555-96-4P
144555-97-5P	144555-98-6P	144555-99-7P	144556-00-3P
144556-01-4P	144556-02-5P	144556-03-6P	**144556-04-7P**
144556-05-8P	144556-06-9P	144556-07-0P	144556-08-1P
144556-09-2P	144556-10-5P	144556-11-6P	144556-12-7P
144556-13-8P	144556-14-9P	**144556-15-0P**	144556-16-1P
144556-17-2P	144556-18-3P	144556-19-4P	144556-20-7P
144556-21-8P	144556-22-9P	144556-23-0P	**144556-24-1P**
144556-25-2P	144556-26-3P	144556-27-4P	144556-28-5P
144556-29-6P	144556-30-9P	144556-31-0P	**144556-32-1P**
144556-33-2P	144556-34-3P	144556-35-4P	144556-36-5P
144556-37-6P	144556-38-7P	144570-22-9P	144570-23-0P
144570-24-1P	144570-25-2P	144570-26-3P	144570-27-4P
144570-28-5P	144570-29-6P	144570-30-9P	144570-31-0P
144570-32-1P	144570-33-2P	144570-34-3P	144570-35-4P
144570-36-5P	144570-37-6P	144570-38-7P	144570-39-8P
144570-40-1P	144570-41-2P	144570-42-3P	144570-43-4P
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144570-48-9P	144570-49-0P	144570-50-3P	144570-51-4P
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144570-68-3P	144570-69-4P	144570-70-7P	144570-71-8P
144570-72-9P	144570-73-0P	144570-74-1P	144570-75-2P
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144570-80-9P	144570-81-0P	144570-82-1P	144570-83-2P
144570-84-3P	144570-85-4P	144570-86-5P	144570-87-6P
144570-88-7P	144570-89-8P	144570-90-1P	144570-91-2P

144570-92-3P 144570-93-4P 144570-94-5P 144570-95-6P
144570-96-7P 144570-97-8P 144570-98-9P 144570-99-0P
144571-00-6P
(prepn. of, as anaphylatoxin receptor ligand)

IT 144571-01-7P 144571-02-8P 144571-03-9P 144571-04-0P
144571-05-1P 144571-06-2P 144571-07-3P 144571-08-4P
144571-09-5P 144571-10-8P 144571-11-9P 144571-12-0P
144571-13-1P 144571-14-2P 144571-15-3P 144571-16-4P
144571-17-5P **144571-18-6P** 144571-19-7P 144571-20-0P
144571-21-1P 144571-22-2P 144571-23-3P 144571-24-4P
144571-25-5P 144596-06-5P 144596-07-6P 144596-08-7P
144596-09-8P 144596-10-1P 144596-11-2P 144596-12-3P
144596-13-4P 144596-14-5P 144596-15-6P 144596-16-7P
144596-17-8P 144596-18-9P 144596-19-0P 144596-20-3P
144596-21-4P 144596-22-5P 144596-23-6P 144596-24-7P
144596-25-8P 144596-26-9P 144596-27-0P 144596-28-1P
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144596-37-2P 144596-38-3P 144596-39-4P **144596-40-7P**
144596-41-8P 144596-42-9P 144596-43-0P 144596-44-1P
144596-45-2P 144596-46-3P 144596-47-4P 144596-48-5P
144596-49-6P 144596-50-9P 144596-51-0P 144596-52-1P
144596-53-2P 144596-54-3P 144596-55-4P 144596-56-5P
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144596-65-6P 144607-88-5P 144607-89-6P **144607-90-9P**
144607-91-0P 144607-92-1P 144607-93-2P 144614-08-4P
144614-09-5P 144614-10-8P 144614-11-9P 144614-12-0P
144614-13-1P 144614-14-2P 144614-15-3P 144614-16-4P
144614-17-5P 144614-18-6P 144614-19-7P 144614-20-0P
144614-21-1P 144614-22-2P 144614-23-3P 144614-24-4P
144614-25-5P 144614-26-6P 144614-27-7P 144614-28-8P
144614-29-9P 144614-30-2P 144614-31-3P 144614-32-4P
144614-33-5P 144614-34-6P 144614-35-7P 144614-36-8P
144614-37-9P 144614-38-0P 144614-39-1P 144614-40-4P
144614-41-5P 144614-42-6P 144614-43-7P 144614-50-6P
144643-97-0P 144644-11-1P 144664-53-9P 144664-54-0P
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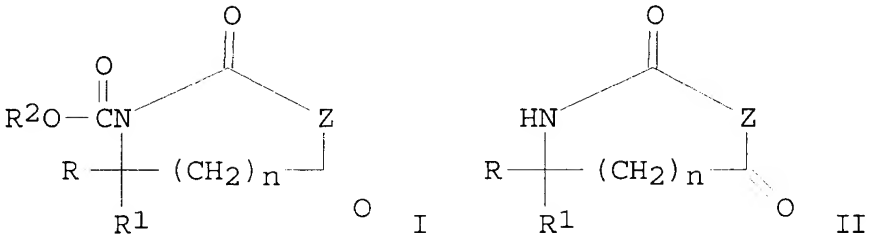
144664-59-5P 144664-60-8P 144664-61-9P 144664-62-0P
144665-63-4P 144665-64-5P 144665-65-6P 144666-79-5P
144666-80-8P 144666-81-9P 144666-82-0P 144666-83-1P
144731-88-4P
(prepn. of, as anaphylatoxin receptor ligand)

IT 144614-47-1P 144614-48-2P 144614-49-3P 144614-51-7P
144643-83-4DP, **resin bound** 144643-86-7DP,
resin bound 144643-87-8DP, **resin**
bound 144643-88-9P 144643-91-4P 144643-92-5P
144643-94-7DP, **resin bound** 144643-95-8P
144643-98-1DP, **resin bound** 144643-99-2DP,
resin bound 144644-02-0P 144644-03-1P
144644-04-2P 144644-05-3P 144644-08-6DP, **resin**
bound 144644-12-2P

(prepn. of, as intermediate for anaphylatoxin receptor ligand)
IT 17609-52-8P **27473-62-7P** 65715-93-7P 78775-63-0P
86778-91-8P 90600-20-7P 144614-45-9P 144614-46-0P
144643-79-8P 144643-80-1P **144643-81-2P** 144643-84-5P
144643-89-0P 144643-96-9P 144644-00-8P 144644-01-9P
144644-06-4P 144644-09-7P 144644-10-0P
(prepn. of, as intermediate for peptide anaphylatoxin receptor ligand)
IT 144614-44-8DP, **resin bound**
(prepn. of, as intermediates for anaphylatoxin receptor ligand)
IT 144643-86-7DP, **resin bound**
(prepn. of, at intermediate for anaphylatoxin receptor ligand)
IT 61315-61-5D, **resin bound**
(reaction of, in prepn. of anaphylatoxin receptor ligand)

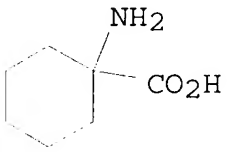
L44 ANSWER 31 OF 36 HCA COPYRIGHT 2003 ACS
115:280578 Urethane-protected amino acid N-carboxy anhydrides. Fuller, William D.; Cohen, Michael P.; Naider, Fred R.; Goodman, Murray (BioResearch, Inc., USA). U.S. US 5028693 A 19910702, 13 pp. Cont. of U.S. 4,946,942. (English). CODEN: USXXAM. APPLICATION: US 1989-379111 19890713. PRIORITY: US 1988-168087 19880311.

GI



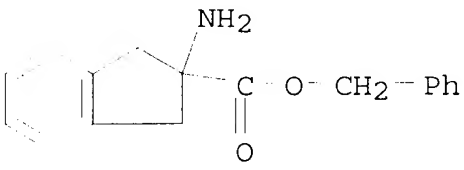
AB The title compds. [I; R, R1 = H, (substituted) alkyl, (substituted) cycloalkyl, (substituted) aryl; R and R1 may not be simultaneously H; R2 = (substituted) alkyl, (substituted) aryl; Z = 0, S; n = 0, 1, 2] are prepd. via reacting an amino acid N-carboxy anhydride or N-thiocarboxy anhydride (II) with R2OC(O)X (X = halo) in an inert solvent contg. a tertiary N-contg. base having an atom or functional group sufficiently electron-rich and positioned relative to the N of the base so as to render said atom or group capable of complexing with the NH group of II or its thio analog but able to generate N-carboxy anhydride or N-thiocarboxy anhydride anionic complexes capable of reacting with the haloformate. Alanine was reacted with phosgene in THF at 62-64% for 4 h and the product in toluene contg. N-methylmorpholine treated with 9-fluorenyl-methoxycarbonyl chloride at 0.degree. for 2 h to give I [Z = O, n = 0, r = Me, R1 = H, R2 = 9-fluorenylmethyl] (III). Leucylalanylvaline was **prepd.** by the **solid phase** method using Fmoc-Val-OH, III, and N-9-fluorenylmethoxycarbonylleucine N-carboxy anhydride.

IT **2756-85-6**
(reaction of, with phosgene)
RN 2756-85-6 HCA
CN Cyclohexanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IC ICM C07K001-00
ICS C07D277-00; C07D279-00; C07D281-00
NCL 530335000
CC 34-3 (Amino Acids, Peptides, and Proteins)
IT 1738-78-9 13734-41-3D, **resin-bound**
(peptide coupling of, with alanine carboxy anhydride deriv.)
IT 68858-20-8D, Fmoc-Val-OH, **resin-bound**
(peptide coupling of, with leucine carboxy anhydride deriv.)
IT 13588-95-9DP, **resin-bound** 123253-88-3DP, **resin-bound**
(prepn. and deprotection-**resin** cleavage of)
IT 61-90-5, Leucine, reactions 63-91-2, Phenylalanine, reactions 72-18-4, Valine, reactions 75-65-0, tert-Butyl alcohol, reactions 2418-95-3 **2756-85-6** 4378-13-6
(reaction of, with phosgene)

L44 ANSWER 32 OF 36 HCA COPYRIGHT 2003 ACS
114:164776 A facile method for the side-chain protection of .alpha.-methyl-.beta.-3,4-dihydroxyphenyl-L-alanine (.alpha.MeDopa) for **solid-phase** peptide **synthesis.**
Hsieh, Kun Hwa; DeMaine, Margaret M. (Dep. Vet. Comp. Anat. Pharmacol. Physiol., Washington State Univ., Pullman, WA, 99164, USA). Synthesis (1), 59-62 (English) 1991. CODEN: SYNTBF. ISSN: 0039-7881.
AB The title compd. was protected as its Me or benzyl esters Boc-L-NHCMe(CH2C6H3R2-3,4)CO2H (I; Boc = Me3CO2C; R = OMe, OCH2Ph) by treatment of I (R = OH) or its Me ester with MeI or PhCH2Cl, followed by sapon. I (R = OCH2Ph) was used in the **solid-phase prepn.** of angiotensin II analogs H-Sar-Arg-Val-.alpha.MeDopa-Val-His-Pro-R1 (R1 = OH, 2-indanecarboxylic acid).
IT **132970-26-4**
(peptide coupling of, with angiotensin II analog)
RN 132970-26-4 HCA
CN 1H-Indene-2-carboxylic acid, 2-amino-2,3-dihydro-, phenylmethyl ester, hydrochloride (9CI) (CA INDEX NAME)

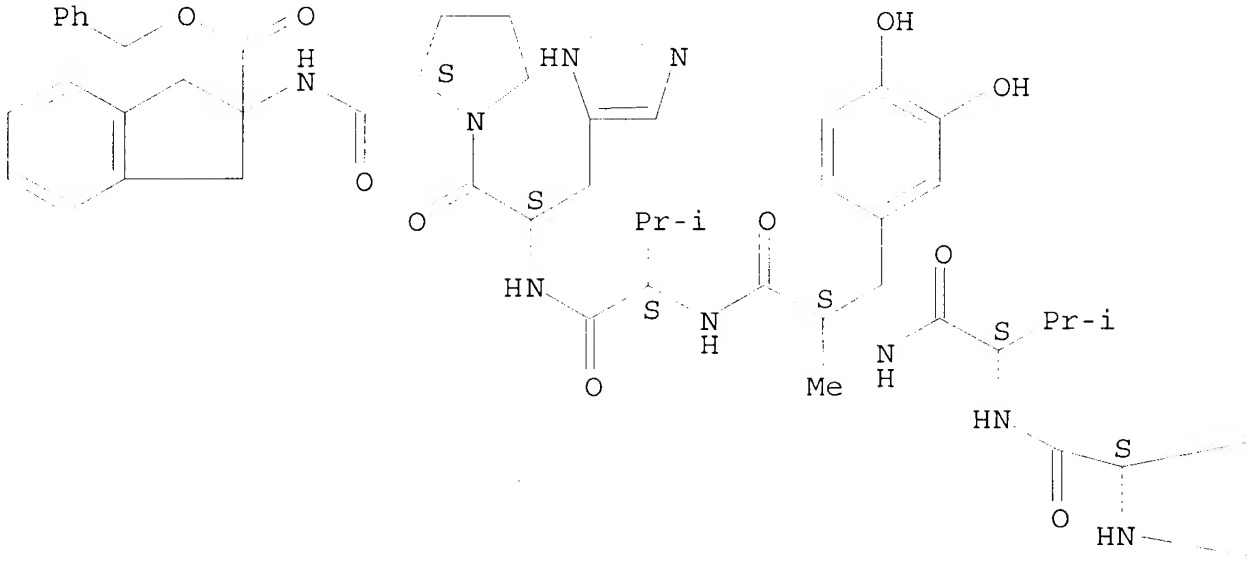


● HCl

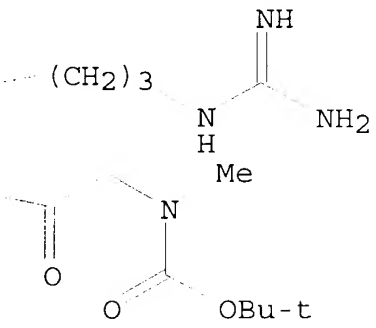
IT **132970-25-3P**
(prepn. and sequential hydrogenolysis and acidic hydrolysis of)
RN 132970-25-3 HCA
CN L-Prolinamide, N-[(1,1-dimethylethoxy)carbonyl]-N-methylglycyl-L-arginyl-L-valyl-3-hydroxy-.alpha.-methyl-L-tyrosyl-L-valyl-L-histidyl-N-[2,3-dihydro-2-[(phenylmethoxy)carbonyl]-1H-inden-2-yl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



CC 34-3 (Amino Acids, Peptides, and Proteins)
IT **132970-26-4**
(peptide coupling of, with angiotensin II analog)
IT 132970-23-1DP, **resin-bound**
(prepn. and hydrogenation-**resin** cleavage of)
IT **132970-25-3P**
(prepn. and sequential hydrogenolysis and acidic hydrolysis of)
IT 132970-21-9P 132970-22-0P
(**prepn**. and **solid-phase** peptide coupling reactions of, angiotensin II analog from)

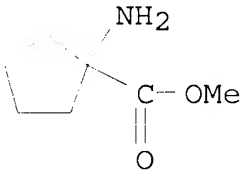
L44 ANSWER 33 OF 36 HCA COPYRIGHT 2003 ACS
108:56613 Amino acids and peptides. Part CCII. Oxytocin analogs with non-coded amino acid residues in position 8: [8-neopentylglycine]oxytocin and [8-cycloleucine]oxytocin. Hlavacek, Jan; Pospisek, Jan; Slaninova, Jirina; Chan, Walter Y.; Hruby, Victor J. (Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10, Czech.). Collection of Czechoslovak Chemical Communications, 52(9), 2317-25 (English) 1987. CODEN: CCCCAK. ISSN: 0366-547X. OTHER SOURCES: CASREACT 108:56613.
GI For diagram(s), see printed CA Issue.
AB Title oxytocin analogs I [X = neopentylglycine (Neo), cycloleucine (Cle)] were prepd. by a combination of solid-phase and fragment condensation methods. Both analogs exhibited decreased uterotonic potency in vitro, each being about 15-30% that of oxytocin (I, X = Leu). I (X = Neo) displayed similarly decreased uterotonic potency

in vivo and galactogogic potency. II (X = Cle) exhibited the same potency as oxytocin in the latter 2 assays.

IT **60421-23-0**
(peptide coupling of, with proline deriv.)

RN 60421-23-0 HCA

CN Cyclopentanecarboxylic acid, 1-amino-, methyl ester, hydrochloride (6CI, 9CI) (CA INDEX NAME)



● HCl

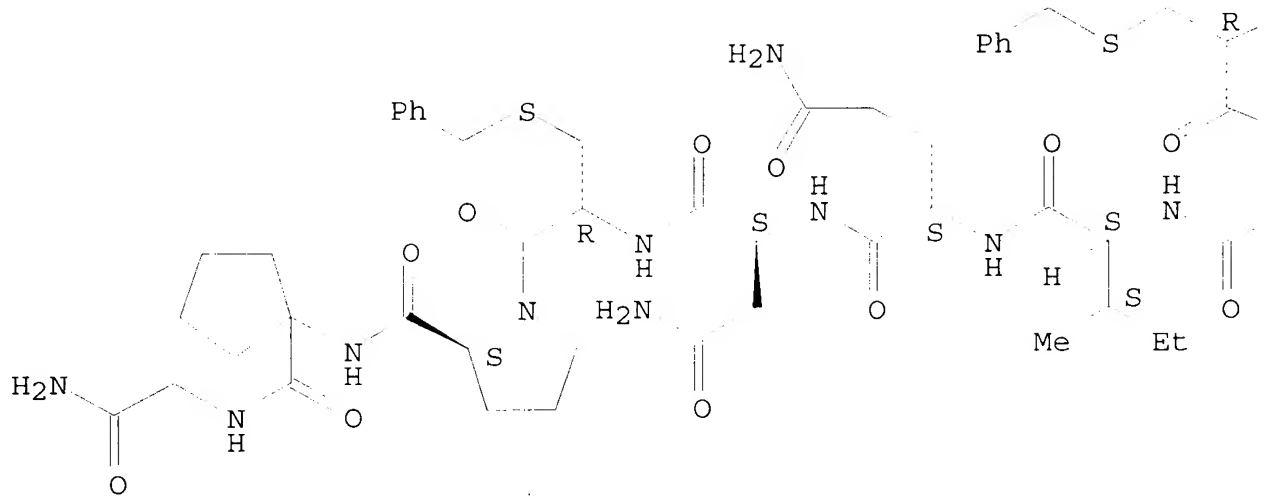
IT **112380-05-9P**
(prepn. and deblocking-oxidative cyclization of)

RN 112380-05-9 HCA

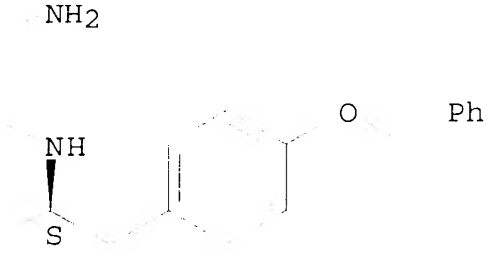
CN Glycinamide, S-(phenylmethyl)-L-cysteinyl-O-(phenylmethyl)-L-tyrosyl-L-isoleucyl-L-glutaminyl-L-asparaginyl-S-(phenylmethyl)-L-cysteinyl-L-prolyl-1-aminocyclopentanecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



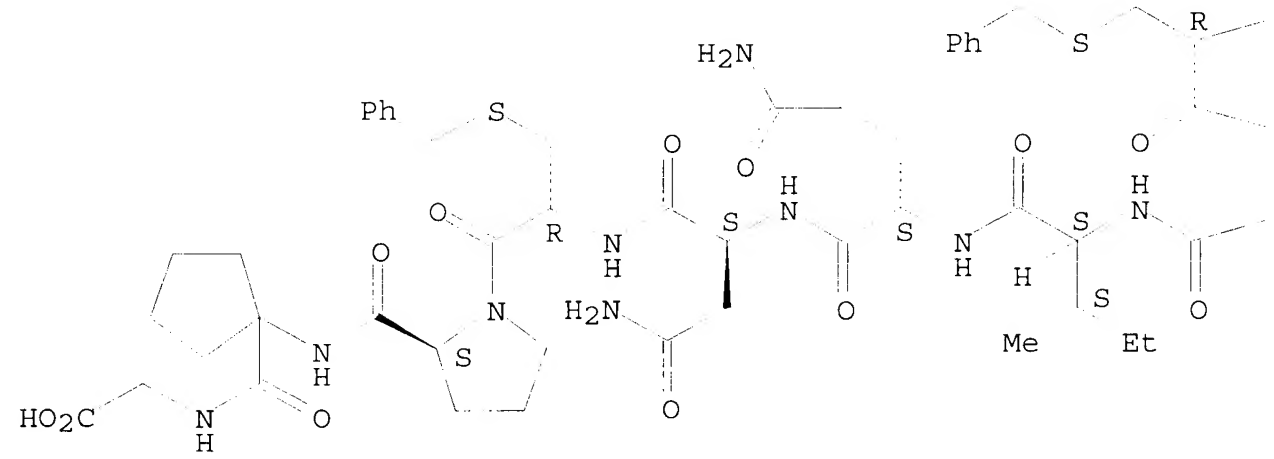
PAGE 1-B



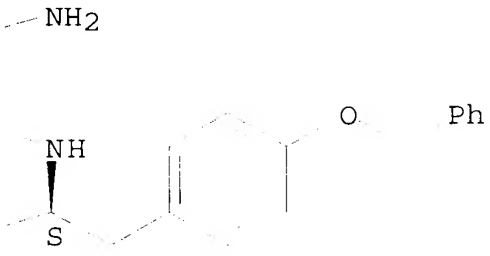
IT **112380-09-3DP, resin-bound**
(prepn. and **resin** cleavage of, by ammonolysis)
RN 112380-09-3 HCA
CN Glycine, S-(phenylmethyl)-L-cysteinyl-O-(phenylmethyl)-L-tyrosyl-L-isoleucyl-L-glutaminyl-L-asparaginyl-S-(phenylmethyl)-L-cysteinyl-L-prolyl-1-aminocyclopentanecarbonyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

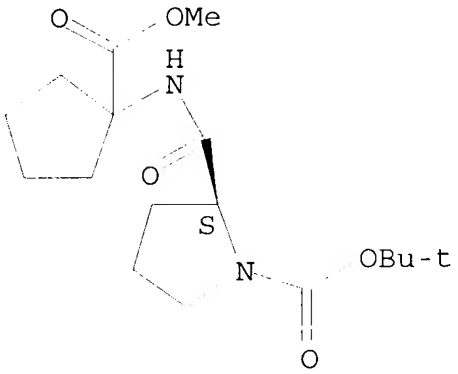


PAGE 1-B



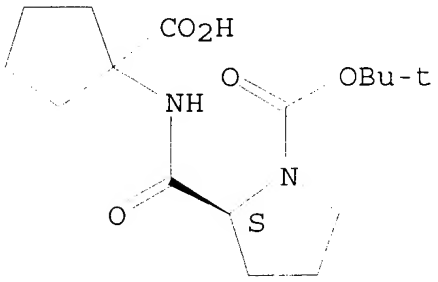
IT **112380-06-0P**
(prepn. and sapon. of)
RN 112380-06-0 HCA
CN 1-Pyrrolidinecarboxylic acid, 2-[[[1-(methoxycarbonyl)cyclopentyl]amino]carbonyl]-, 1,1-dimethylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **112380-07-1P**
(**prepn**. and **solid-phase** peptide coupling of)
RN 112380-07-1 HCA
CN 1-Pyrrolidinecarboxylic acid, 2-[[(1-carboxycyclopentyl)amino]carbonyl]-, 1-(1,1-dimethylethyl) ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **112380-02-6P 112380-03-7P**
(prepn. and uterotonic and galactogogic activities of)
RN 112380-02-6 HCA
CN Oxytocin, 8-(1-aminocyclopentanecarboxylic acid)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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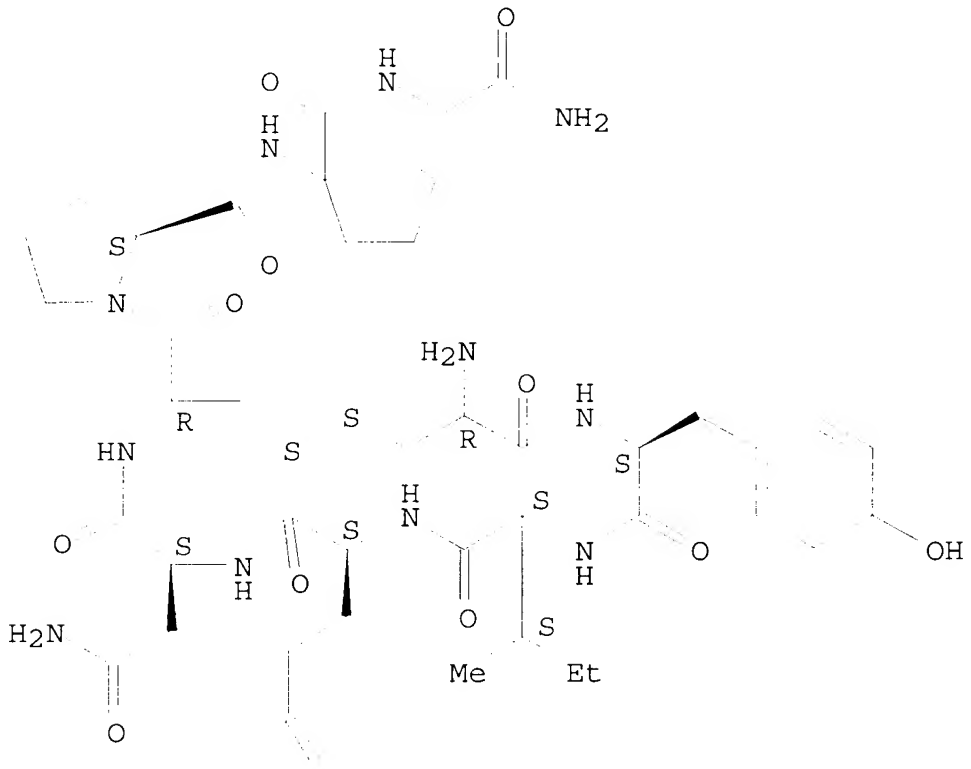

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RN 112380-03-7 HCA
CN Oxytocin, 8-(1-aminocyclopentanecarboxylic acid)-, monoacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 112380-02-6
CMF C43 H64 N12 O12 S2

Absolute stereochemistry.

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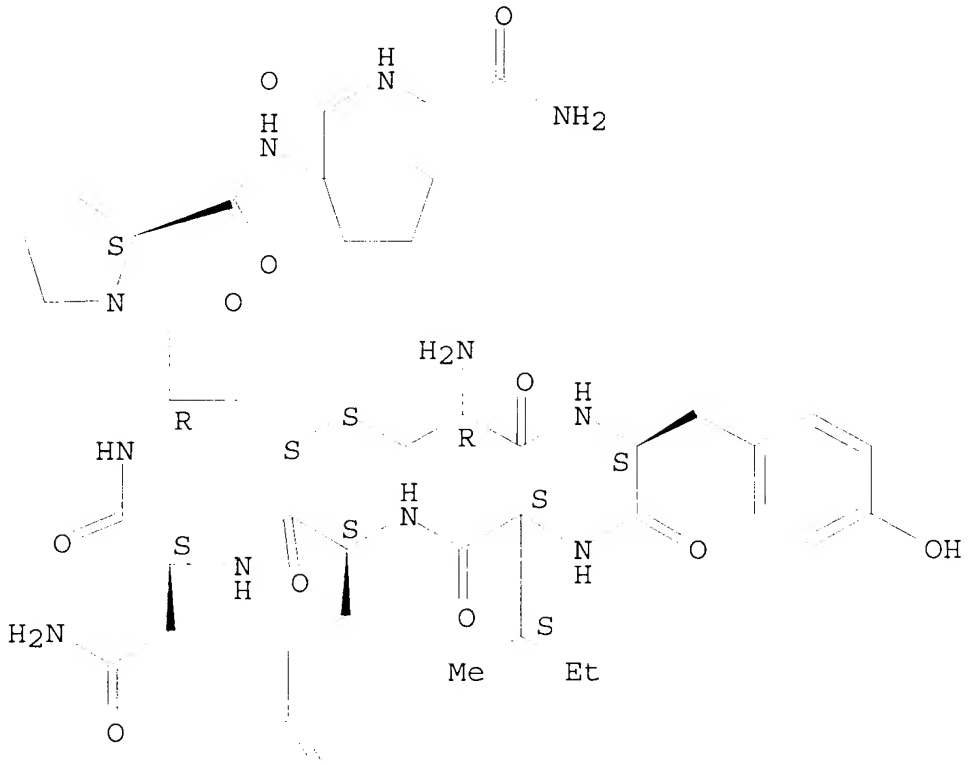

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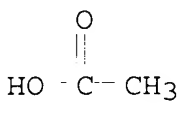
CM 2

CRN 64-19-7
CMF C2 H4 O2



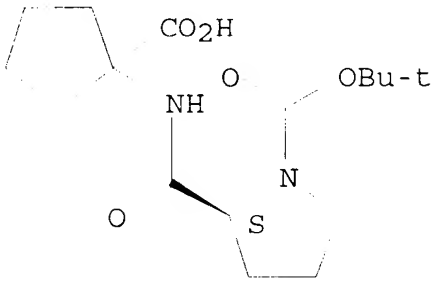
IT **112380-08-2P**
(prepn. of)
RN 112380-08-2 HCA

CN 1-Pyrrolidinecarboxylic acid, 2-[[(1-carboxycyclopentyl)amino]carbonyl]-, mono(1,1-dimethylethyl) ester, (S)-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

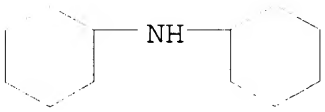
CRN 112380-07-1
CMF C16 H26 N2 O5

Absolute stereochemistry.



CM 2

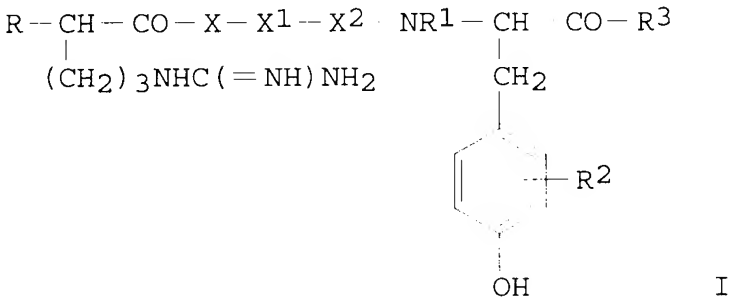
CRN 101-83-7
CMF C12 H23 N



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 2
IT **60421-23-0**
(peptide coupling of, with proline deriv.)
IT 112380-04-8P **112380-05-9P**
(prepn. and deblocking-oxidative cyclization of)
IT 98477-21-5DP, **resin-bound**
(prepn. and **resin** cleavage of)
IT **112380-09-3DP**, **resin-bound**
(prepn. and **resin** cleavage of, by ammonolysis)
IT **112380-06-0P**
(prepn. and sapon. of)
IT **112380-07-1P**
(**prepn**. and **solid-phase** peptide coupling of)
IT 50-56-6DP, Oxytocin, non-coated amino acid-contg. analogs
50-56-6P, preparation 112380-01-5P **112380-02-6P**
112380-03-7P

(prepn. and uterotonic and galactogogic activities of)
IT **112380-08-2P**
(prepn. of)
IT 4530-20-5D, N-(tert-Butoxycarbonyl)glycine, **resin-bound** 5068-28-0D, **resin-bound**
(**solid-phase** peptide **synthesis** with)

L44 ANSWER 34 OF 36 HCA COPYRIGHT 2003 ACS
104:19821 Enzyme-resistant immunomodulatory peptides. Goldstein, Gideon; Heavner, George; Kroon, Daniel; Audhya, Tapan (Ortho Pharmaceutical Corp., USA). U.S. US 4505853 A 19850319, 20 pp. (English). CODEN: USXXAM. APPLICATION: US 1983-553281 19831118.
GI

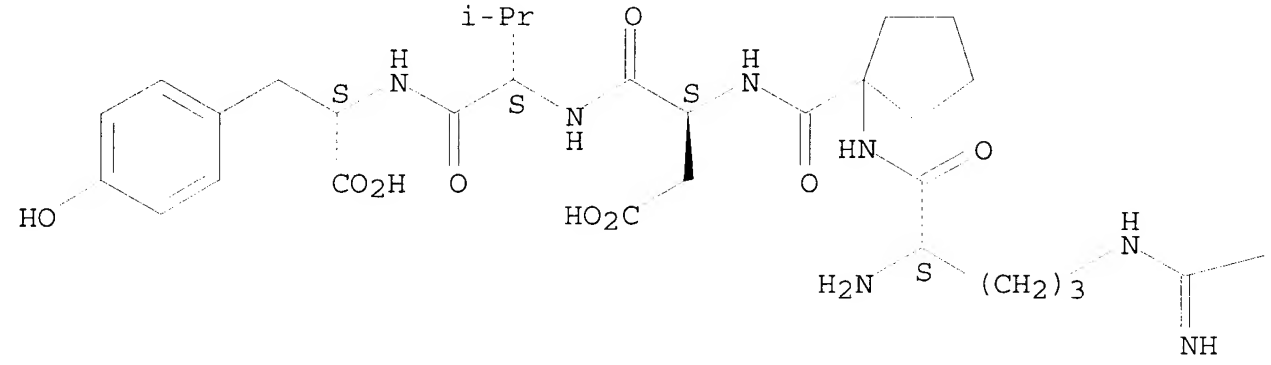


I

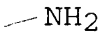
AB Thymopoietin-like peptides I [R = H, NH2, aclamino, MeNH, pyroglutamylamino; X = Pro, dehydroprolyl, NHCR4R5CO (R4, R5 = alkyl); X1 = D-Asp, Asp, D-Glu, Glu; X2 = Gly, Val, Leu, Nle, Phe, Ile, Lys, Gln, Glu, Ala, D-Val, D-Leu, D-Nle, D-Phe, D-Ile, D-Lys, D-Gln, D-Glu, D-Ala; R1 = H, alkyl; R2 = H, group which increases phenolic proton acidity; R3 = OH, NH2, alkylamino, NHCHR4CO2H or NHCHR4CONHR5 (R4, R5 = H, alkyl)] were prepd. as immunomodulating agents with great resistance to degrdn. by peptidases. Thus, Ac-Arg-Pro-Asp-Val-Tyr-NH2 (II) was **prepd.** by the **solid-phase** method on a p-methylbenzhydrylamine resin. II required >1400 min for 50% degrdn. by leucine aminopeptidase (LAP), whereas thymopentin underwent 50% degrdn. by LAP in only 15 min.
IT **99460-27-2P**
(prepn. and stability of, to peptidases)
RN 99460-27-2 HCA
CN L-Tyrosine, L-arginyl-1-aminocyclopentanecarbonyl-L-.alpha.-aspartyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

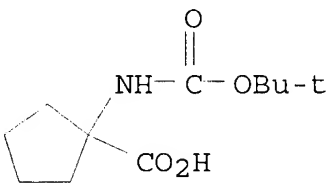
PAGE 1-A



PAGE 1-B



IT **35264-09-6**
(solid-phase peptide coupling of)
RN 35264-09-6 HCA
CN Cyclopentanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]-
(9CI) (CA INDEX NAME)



IC ICM C07C103-52
ICS A61K037-00
NCL 260112500R
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 7, 15
IT 99459-75-3P 99459-83-3DP, **resin-bound**
(prepn. and partial deblocking-N-acetylation of)
IT 99459-69-5DP, p-methylbenzhydrylamine **resin-bound**
99459-79-7DP, **resin-bound** 99459-81-1DP,

resin-bound 99459-86-6DP, **resin-bound** 99460-19-2DP, p-methylbenzhydrylamine **resin-bound**
(prepn. and **resin** cleavage-deblocking of)
IT 51154-06-4P
(**prepn**. and **solid-phase** peptide coupling of)
IT 81189-61-9DP, **resin-bound**
(**prepn**. and **solid-phase** peptide **synthesis** with)
IT 99109-44-1P 99459-68-4P 99460-21-6P 99460-23-8P 99460-26-1P **99460-27-2P** 99528-70-8P
(prepn. and stability of, to peptidases)
IT 99459-85-5DP, **resin-bound** 99460-02-3P 99460-14-7P
(prepn. and N-acetylation of)
IT 7536-58-5 13139-16-7 13574-13-5 13734-34-4 13734-41-3 15387-45-8 15761-39-4 31948-52-4 **35264-09-6**
(solid-phase peptide coupling of)
IT 40298-71-3D, **resin-bound** 47689-67-8D, **resin-bound** 99460-28-3D, **resin-bound**
(**solid-phase** peptide **synthesis** with)

L44 ANSWER 35 OF 36 HCA COPYRIGHT 2003 ACS
93:24113 Further studies on the structural requirements for synthetic peptide chemoattractants. Freer, Richard J.; Day, Alan R.; Radding, Jeffrey A.; Schiffmann, Elliott; Aswanikumar, S.; Showell, Henry J.; Becker, Elmer L. (Dep. Pharmacol., Med. Coll. Virginia, Richmond, VA, 23298, USA). Biochemistry, 19(11), 2404-10 (English) 1980. CODEN: BICHAW. ISSN: 0006-2960.
AB Thirty small mol. wt. peptides related to the chemotactic peptide N-formylmethionylleucylphenylalanine (I) were **prepd**. by both **solid-phase** and classical peptide **synthesis**. Compds. were prepd. to investigate the structural requirements in the 1 position (N-formylmethionine) and the 3 position (phenylalanine). Each analog was tested for its ability to induce lysosomal enzyme release from cytochalasin B-treated rabbit polymorphonuclear leukocytes in vitro. In addn., some also were tested for their ability to stimulate neutrophil chemotaxis in vitro and for inhibition of specific binding of a 3H-labeled chemotactic peptide, CHO-Nle-Leu-Phe-OH (CHO = N-formyl). The formyl group of I is essential for good biol. activity since N-acetylation, removal of the .alpha.-amino group (i.e., desamino), or replacement by an Et group results in a drastic loss of chemotactic potency (.apprx.5000-fold). In addn., the S-contg. side chain of methionine produces optimum activity of the tripeptide. Analogs contg. other S-contg. amino acids (ethionine, methylcysteine) were less active, as were a variety of analogs contg. linear aliph., arom., or branched aliph. side chains at position 1. A limited no. of analogs were prepd. to probe

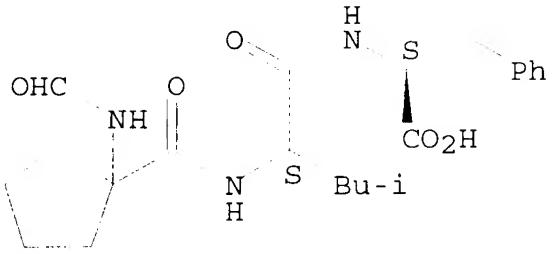
structure-activity relation at position 3. The primary sequence, Met-Leu-Phe, generates the most active chemoattractants, although addn. of a large, highly charged lysine residue allowed the retention of a large degree of chemotactic activity. A free COOH group may be desirable, however, since CHO-Met-Leu-.beta.-phenylethylamine (descarboxy-Phe) is relatively inactive. Finally, several related compds. were identified which are specific competitive antagonists of I-induced lysosomal enzyme release and chemotaxis.

IT **73572-49-3P**
(prepn. and chemotactic activity of)

RN 73572-49-3 HCA

CN L-Phenylalanine, N-[N-[[1-(formylamino)cyclopentyl]carbonyl]-L-leucyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 15-2 (Immunochemistry)

IT 26055-05-0P 59880-97-6P 59881-08-2P 61864-82-2P 61864-83-3P
67247-11-4P 67247-12-5P 73572-34-6P 73572-35-7P 73572-36-8P
73572-37-9P 73572-38-0P 73572-39-1P 73572-40-4P 73572-41-5P
73572-42-6P 73572-43-7P 73572-44-8P 73572-45-9P 73572-46-0P
73572-47-1P 73572-48-2P **73572-49-3P** 73572-50-6P
73572-51-7P 73572-52-8P 73572-53-9P 73572-54-0P 73572-55-1P
73572-56-2P 73572-57-3P 73572-58-4P
(prepn. and chemotactic activity of)

L44 ANSWER 36 OF 36 HCA COPYRIGHT 2003 ACS

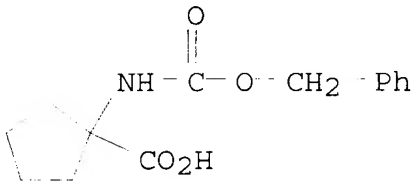
82:98368 **Solid-phase** peptide **synthesis** of 1-aminocyclopentanecarboxylic acid (ACPC) analogs of angiotensin II using a new apparatus. Park, Won K.; Asselin, J.; Berlinguet, L. (Fac. Med., Laval Univ., Quebec, QC, Can.). Prog. Pept. Res., [Proc. Am. Pept. Symp.], 2nd, Meeting Date 1970, 49-58. Editor(s): Lande, Saul. Gordon and Breach: New York, N. Y. (English) 1972. CODEN: 29USAB.

AB AC-PC-Arg-Val-Tyr-Ile-His-Pro-Phe, Asp-Arg-ACPC-Tyr-Ile-His-Pro-Phe, Asp-Arg-Val-Tyr-Ile-ACPC-Pro-Phe, Asp-Arg-Val-Tyr-Ile-His-ACPC-Phe, and Asp-Arg-Val-Tyr-Ile-His-Pro-ACPC, with 40, 1.0-2.0, 0.1-0.5, 1.0-1.5, and 0.1-0.5%, resp., of the pressor activity of (1-Asp, 5-Ile) angiotensin II, were prepd. in 51-55% yield from the N-tert-butoxycarbonyl blocked amino acids using the manual valving system app. described for **solid phase** peptide

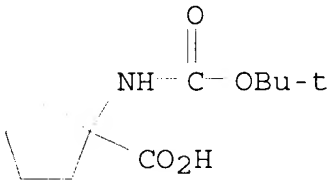
synthesis.

IT **17191-44-5P 35264-09-6P 55260-18-9P**
(prepn. and peptide coupling reactions of)

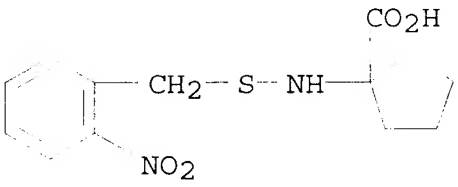
RN 17191-44-5 HCA
CN Cyclopentanecarboxylic acid, 1-[[(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 35264-09-6 HCA
CN Cyclopentanecarboxylic acid, 1-[[(1,1-dimethylethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

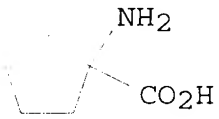


RN 55260-18-9 HCA
CN Cyclopentanecarboxylic acid, 1-[[[(2-nitrophenyl)methyl]thio]amino]- (9CI) (CA INDEX NAME)



IT **52-52-8P**
(prepn. and peptide coupling reactions of, angiotensin II anal. contg.)

RN 52-52-8 HCA
CN Cyclopentanecarboxylic acid, 1-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



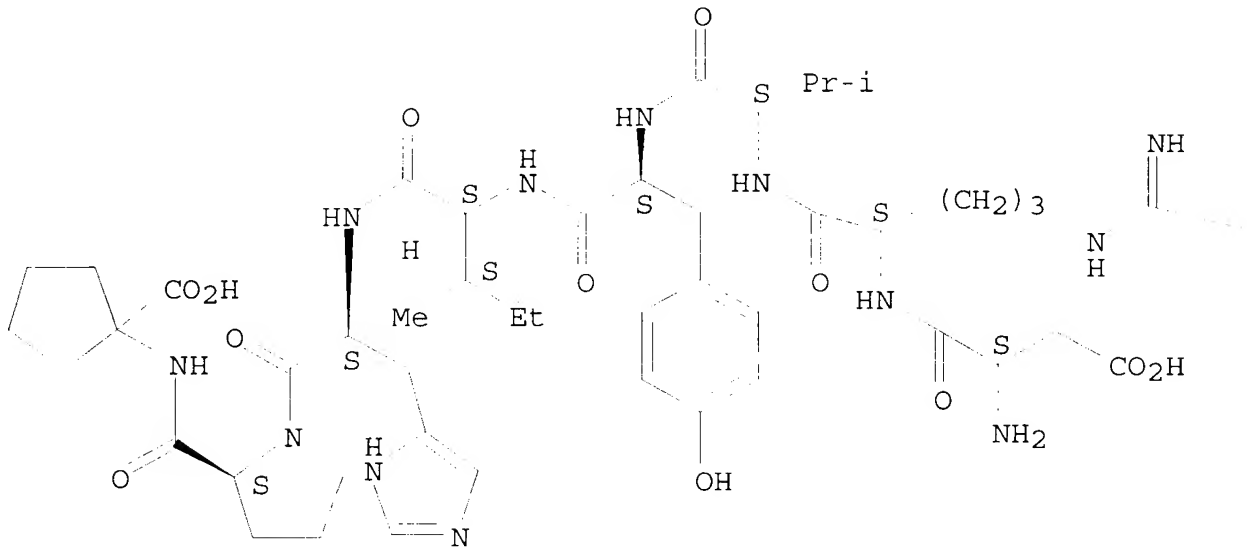
IT **34409-25-1P 37578-26-0P 37589-45-0P 37635-78-2P**
(**solid phase prepn.** of and pressor activity of)

RN 34409-25-1 HCA

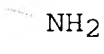
CN L-Prolinamide, L-.alpha.-aspartyl-L-arginyl-L-valyl-L-tyrosyl-L-isoleucyl-L-histidyl-N-(1-carboxycyclopentyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

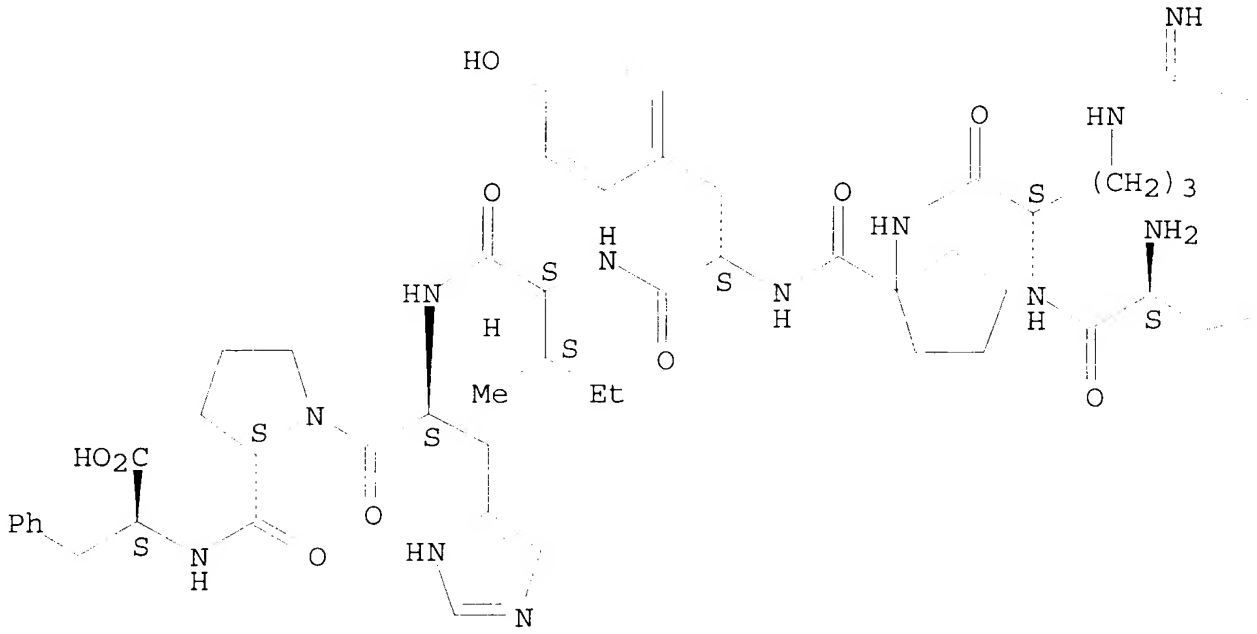


RN 37578-26-0 HCA

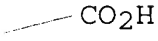
CN Angiotensin II, 3-(1-aminocyclopentanecarboxylic acid)-5-L-isoleucine- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

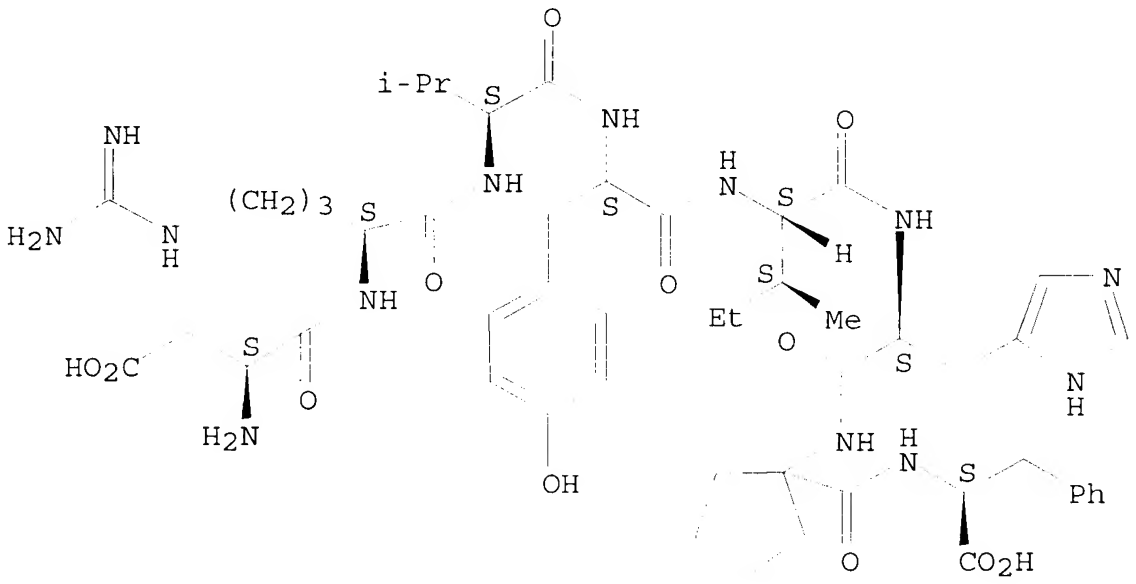


PAGE 1-B



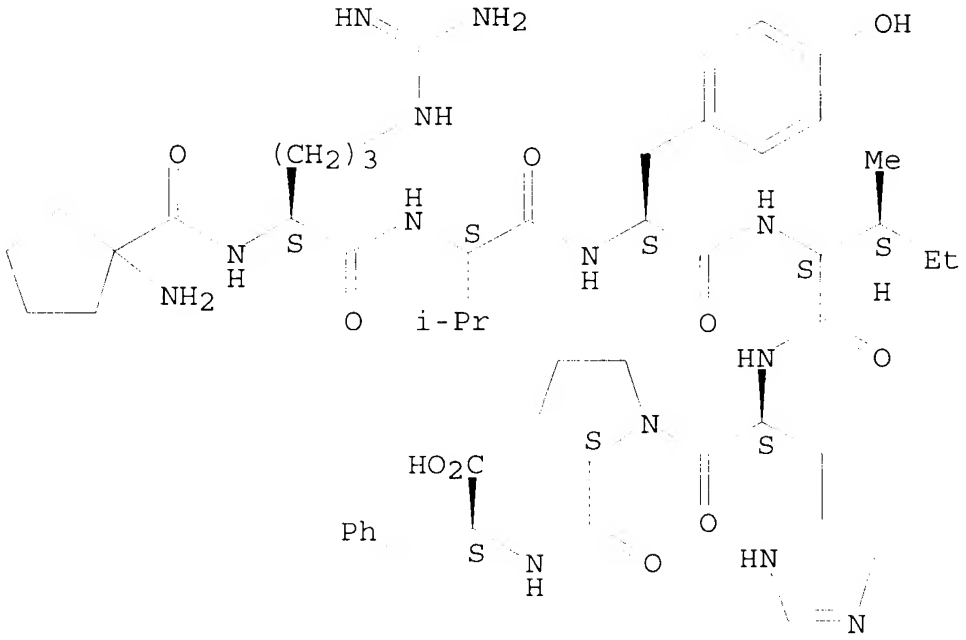
RN 37589-45-0 HCA
CN Angiotensin II, 5-L-isoleucine-7-(1-aminocyclopentanecarboxylic acid)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 37635-78-2 HCA
CN Angiotensin II, 1-(1-aminocyclopentanecarboxylic acid)-5-L-isoleucine- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 34-3 (Synthesis of Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 1
IT Peptides, **preparation**
(**solid-phase**, app. for)
IT **17191-44-5P 35264-09-6P 55260-18-9P**
(prepn. and peptide coupling reactions of)
IT **52-52-8P**
(prepn. and peptide coupling reactions of, angiotensin II anal. contg.)
IT **34409-25-1P** 37574-62-2P **37578-26-0P**
37589-45-0P 37635-78-2P
(**solid phase prepn**. of and pressor activity of)

=> d l45 1-60 ti

L45 ANSWER 1 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of 3-amino-3-phenylpropanoic acid amino acid derivatives as inhibitors of integrin .alpha.v.beta.6

L45 ANSWER 2 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of triazaspiro[5.5]undecane derivatives as the active ingredients useful in prevention or as remedy for HIV infection

L45 ANSWER 3 OF 60 HCA COPYRIGHT 2003 ACS
TI Peptides with indirect in vivo activity against an intracellular pathogen: selective lysis of infected macrophages

L45 ANSWER 4 OF 60 HCA COPYRIGHT 2003 ACS
TI Synthesis and receptor binding of oxytocin analogs containing conformationally restricted amino acids

L45 ANSWER 5 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of amino acid derivatives for modulating angiotensin converting enzyme-2 (ACE-2)

L45 ANSWER 6 OF 60 HCA COPYRIGHT 2003 ACS
TI Design and Synthesis of a Fluorescent Reporter of Protein Kinase Activity

L45 ANSWER 7 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of peptides as melanocortin receptor ligands

L45 ANSWER 8 OF 60 HCA COPYRIGHT 2003 ACS
TI TOAC: The rigid nitroxide side chain

L45 ANSWER 9 OF 60 HCA COPYRIGHT 2003 ACS
TI A simple synthesis of [11C]carfentanil using an extraction disk instead of HPLC

L45 ANSWER 10 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of cyclic peptides having melanocortin-4 receptor

(MC4-R) agonist activity

L45 ANSWER 11 OF 60 HCA COPYRIGHT 2003 ACS
TI Therapeutic azo group-containing polyanhydrides for drug delivery

L45 ANSWER 12 OF 60 HCA COPYRIGHT 2003 ACS
TI Therapeutic polyanhydride compounds for drug delivery

L45 ANSWER 13 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of substance P analogs for the treatment of cancer

L45 ANSWER 14 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of somatostatin analogs for the treatment of cancer

L45 ANSWER 15 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of selective linear peptides with melanocortin-4 receptor (MC4-R) agonist activity

L45 ANSWER 16 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of peptides which inhibit human tissue kallikrein and the liberation of kinins

L45 ANSWER 17 OF 60 HCA COPYRIGHT 2003 ACS
TI Synthesis of bombesin peptide analogs and their uses in treatment of cancer

L45 ANSWER 18 OF 60 HCA COPYRIGHT 2003 ACS
TI Crystal structure of CDC25 proteins and its use in rational design of inhibitors

L45 ANSWER 19 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of N.alpha.-benzyloxycarbonyl-N-(2-anilinoethyl)leucineamides and analogs as cathepsin K inhibitors

L45 ANSWER 20 OF 60 HCA COPYRIGHT 2003 ACS
TI A Rational Approach to the Design and Synthesis of a New Bradykinin B1 Receptor Antagonist

L45 ANSWER 21 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of N-acylphenylalanine derivatives and analogs as inhibitors of .alpha.4.beta.1 mediated cell adhesion

L45 ANSWER 22 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of glucagon-like peptide-1 (GLP-1) analogs

L45 ANSWER 23 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of glucagon-like peptide-1 (GLP-1) analogs

L45 ANSWER 24 OF 60 HCA COPYRIGHT 2003 ACS
TI Synthesis of Indan-Based Unusual .alpha.-Amino Acid Derivatives under Phase-Transfer Catalysis Conditions

L45 ANSWER 25 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of C-terminal modified oxamyl dipeptides as inhibitors of the ICE/ced-3 family of cysteine proteases

L45 ANSWER 26 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of Technetium-99m labeled peptides for imaging inflammation

L45 ANSWER 27 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of parathyroid hormone analogs

L45 ANSWER 28 OF 60 HCA COPYRIGHT 2003 ACS
TI An investigation of position 3 in arginine vasopressin with aliphatic, aromatic, conformationally-restricted, polar and charged amino acids

L45 ANSWER 29 OF 60 HCA COPYRIGHT 2003 ACS
TI New chimeric analogs of galanin: synthesis and effects on the glucose-induced insulin secretion

L45 ANSWER 30 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of linear dolastatin peptides as antitumor agents

L45 ANSWER 31 OF 60 HCA COPYRIGHT 2003 ACS
TI Microwave-Mediated Intramolecular Carbanilide Cyclization to Hydantoins Employing Barium Hydroxide Catalysis

L45 ANSWER 32 OF 60 HCA COPYRIGHT 2003 ACS
TI Incorporation of .alpha.-substituted serine analog into peptide via a novel O,N-migration

L45 ANSWER 33 OF 60 HCA COPYRIGHT 2003 ACS
TI Synthesis of conformationally constrained .alpha.-amino acid derivatives using ethyl isocyanoacetate as glycine equivalent

L45 ANSWER 34 OF 60 HCA COPYRIGHT 2003 ACS
TI Imidazole-containing benzodiazepines and analogs as inhibitors of farnesyl protein transferase

L45 ANSWER 35 OF 60 HCA COPYRIGHT 2003 ACS
TI Antagonists of LHRH

L45 ANSWER 36 OF 60 HCA COPYRIGHT 2003 ACS
TI Synthesis of a series of polar, orthogonally protected, .alpha.,.alpha.-disubstituted amino acids

L45 ANSWER 37 OF 60 HCA COPYRIGHT 2003 ACS
TI 2,4-Methano amino acids, novel constituents of bioactive peptides: tuftsin as a model

L45 ANSWER 38 OF 60 HCA COPYRIGHT 2003 ACS
TI Acylated oligopeptide derivatives having cell signal inhibiting

activity

L45 ANSWER 39 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of meta-guanidine, urea, thiourea or azacyclic amino benzoic acid derivatives as integrin antagonists

L45 ANSWER 40 OF 60 HCA COPYRIGHT 2003 ACS
TI Acylated oligopeptides containing phosphotyrosine as inhibitors of protein tyrosine kinases

L45 ANSWER 41 OF 60 HCA COPYRIGHT 2003 ACS
TI Use of spin label EPR spectra to monitor peptide chain aggregation inside resin beads

L45 ANSWER 42 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of peptides and compounds that bind to SH2 (src homology region 2) domains of proteins and methods for their identification

L45 ANSWER 43 OF 60 HCA COPYRIGHT 2003 ACS
TI Antimicrobial .alpha.,.alpha.-Dialkylated Amino Acid Rich Peptides with in-Vivo Activity against an Intracellular Pathogen

L45 ANSWER 44 OF 60 HCA COPYRIGHT 2003 ACS
TI Synthesis and Characterization of Pseudopeptide Bradykinin B2 Receptor Antagonists Containing the 1,3,8-Triazaspiro[4.5]decan-4-one Ring System

L45 ANSWER 45 OF 60 HCA COPYRIGHT 2003 ACS
TI Protein Structure-Based Design of Combinatorial Libraries: Discovery of Non-Peptide Binding Elements to Src SH3 Domain

L45 ANSWER 46 OF 60 HCA COPYRIGHT 2003 ACS
TI Asymmetric syntheses of the stereoisomers of protected 2,3-methanoglutamine

L45 ANSWER 47 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of peptides cyclized to tetrahydronaphthalene moieties as research tools (models of protein .alpha.-helicity) and as potential drugs.

L45 ANSWER 48 OF 60 HCA COPYRIGHT 2003 ACS
TI Analogs of parathyroid hormone

L45 ANSWER 49 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of lipid conjugates of therapeutic peptides and protease inhibitors

L45 ANSWER 50 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of modified peptides transportable into the central nervous system

L45 ANSWER 51 OF 60 HCA COPYRIGHT 2003 ACS

TI Substrate specificity of isopenicillin N synthase

L45 ANSWER 52 OF 60 HCA COPYRIGHT 2003 ACS
TI Ring substituted and other conformationally constrained tyrosine analogs of [cyclic] [D-Pen2,D-Pen5]enkephalin with .delta.-opioid receptor selectivity

L45 ANSWER 53 OF 60 HCA COPYRIGHT 2003 ACS
TI Conformational restriction of the phenylalanine residue in a cyclic opioid peptide analog: effects on receptor selectivity and stereospecificity

L45 ANSWER 54 OF 60 HCA COPYRIGHT 2003 ACS
TI Preparation of peptides as inhibitors of protein-platelet adhesion, cell-cell adhesion, and platelet aggregation

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TI Atrial natriuretic polypeptide derivatives as drugs

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TI Preparation of urethane-protected amino acid N-carboxy anhydrides

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TI Receptor-bound conformation of peptides: morphiceptin

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TI Pharmacological, conformational and dynamic properties of cycloleucine-2 analogs of oxytocin and [1-penicillamine]oxytocin

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TI Synthesis, biological activity and resistance to enzymic degradation of luteinizing hormone-releasing hormone analogs modified at position 7

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TI Angiotensin II analogs. 12. Role of the aromatic ring of position 8 phenylalanine in pressor activity